Enhancing particle number concentration modelling accuracy in China by incorporating various nucleation parameterization schemes into the CMAQ version 5.3.2 model

Jianjiong Mao[1,2], Lei Jiang[1], Zhicheng Feng[1], Jingyi Li[1], Yanhong Zhu[1], Momei Qin[1], Song Guo[2,3], Min Hu[2,3], Jianlin Hu[1,3]

[1] Jiangsu Key Laboratory of Atmospheric Environment Monitoring and Pollution Control, School of Environmental Science and Engineering, Nanjing University of Information Science & Technology, Nanjing 210044, China

[2] State Key Laboratory of Regional Environment and Sustainability, International Joint Laboratory for Regional Pollution Control, Ministry of Education (IJRC), College of Environmental Sciences and Engineering, Peking University, Beijing 100871, China

[3] Collaborative Innovation Center of Atmospheric Environment and Equipment Technology, Nanjing University of Information Science & Technology, Nanjing 210044, China

Correspondence to: Jianlin Hu (jianlinhu@nuist.edu.cn)

Abstract. Particle number concentration (PNC) is a key parameter for assessing particles' effects on public health and climate. Although the Community Multiscale Air Quality (CMAQ) model has been widely used to investigate the particle mass concentrations in China, its capability of reproducing the PNC is unclear. After applying the default CMAQ model (version 5.3.2) in Beijing and Nanjing, the model underestimates PNC by 70% to 80% with the default Binary Homogeneous Nucleation (BHN) parameterization scheme. We then implement Ternary Homogeneous Nucleation (THN), Ion Mediated Nucleation (IMN), and sulfuric acid-dimethylamine (DMA) nucleation parameterization schemes into the CMAQ model. Seven modelling scenarios are conducted to explore the model's performance on PNC. The results indicate that the scenario with combined IMN and DMA scheme (SumID scheme) yields the best agreement with the observations, enhancing PNC during new particle formation (NPF) events by 84% in Beijing and 36% in Nanjing. In SumID scheme, IMN contributes to 56.30% of the number concentrations in Beijing and 27.86% in Nanjing, while DMA accounts for 28.15% in Beijing and 29.27% in Nanjing, respectively. IMN nucleation contributed PNC exhibits a pronounced diurnal variation with higher concentrations during the day and lower levels at night. DMA pathway predominantly influences NPF events during the morning and evening peak. This study enhances the model's capability to accurately simulate NPF events and underscores the significant influence of IMN and DMA nucleation on PNC in eastern cities.

***Keywords**:* New particle formation; nucleation parameterization; number concentration; ion mediated nucleation; sulfuric acid-dimethylamine nucleation.

Synopsis: CMAQ model incorporated with IMN and DMA nucleation schemes significantly improves its modeling accuracy for particle number concentrations in eastern cities.

1. Introduction

Particulate matter (PM) significantly impacts regional air quality (Fuzzi et al., 2015), global climate change (Ning et al., 2024; Zhang et al., 2024), and public health (Hu et al., 2017a). Particle number concentration (PNC) is a critical parameter for assessing its environmental health and climate impacts. New particle formation (NPF), a process in which gaseous vapors in the atmosphere form critical molecular clusters that grow into particles (Zhang et al., 2012; Wang et al., 2017), is a significant source of PNC, contributing ~30% of PNC at the surface and over 90% in the upper troposphere (Yu et al., 2020b; Zhao et al., 2024).

Laboratory and ambient observational studies have been conducted in various locations and environments to investigate the NPF processes. Sulfuric acid (H_2SO_4), ammonia (NH_3), ion, organic vapors, dimethylamine, nitric acid (HNO_3), and iodic acid (HIO_3)/iodous acid (HIO_2) are found to participate in the particle nucleation. A few nucleation theories and parameterizations have been proposed, such as H_2SO_4-water (H_2O) Binary Homogeneous Nucleation (BHN) (Kulmala et al., 1998; Vehkamäki, 2002; Yu, 2006a, 2007), H_2SO_4-NH_3-H_2O Ternary Homogeneous Nucleation (THN) (Napari, 2002; Napari et al., 2002; Merikanto et al., 2007; Almeida et al., 2013), Ion Induced Nucleation (IIN) (Laakso, 2002; Liu et al., 2022), Ion Mediated Nucleation (IMN) (Yu and Turco, 1997, 2000, 2001; Yu, 2002, 2006b, 2010; Yu et al., 2008; Yu et al., 2010; Yu et al., 2018; Yu et al., 2020a), H_2SO_4-dimethylamine nucleation (DMA) (Loukonen et al., 2010; Kurten et al., 2014; Ruusuvuori et al., 2015; Olenius et al., 2017; Julin et al., 2018; Lu et al., 2020; Liu et al., 2021a; Liu et al., 2021b; Wang et al., 2021b), organic nucleation (Zhang et al., 2004; Fan et al., 2006; Wang et al., 2015; Yan et al., 2021), HNO_3-H_2SO_4-NH_3 nucleation (Wang et al., 2022b) and HIO_3/HIO_2 nucleation (Zhang et al., 2022; Zhao et al., 2024). Different nucleation theories are applicable to various environments, and multiple nucleation theories are interrelated and nucleate synergistically in some cases. For example, the IMN theory takes into account BHN, as well as the synergistic effects between THN and ions (Yu et al., 2018; Yu et al., 2020a).

Based on these studies, various nucleation parameterization schemes, which calculate nucleation rates based on precursor concentrations and environmental factors, have been developed and implemented into three-dimensional (3-D) chemical transport models (CTMs) to study NPF events or PNC in the atmosphere. The WACCM model shows that BHN underestimates number concentration in the upper

troposphere and lower stratosphere (English et al., 2011). The GEOS-Chem-APM model, utilizing the IMN parameters, suggests that IMN predominantly influences PNC in the troposphere (Yu et al., 2010). The NAQPMS-APM-VBS model demonstrates that organic nucleation can reproduce the summer NPF events in Beijing (Chen et al., 2019). By coupling all the different forms of nucleation parameterization schemes discussed above, the E3SM model indicates that H_2SO_4-dimethylamine nucleation dominates number concentration in 1 km height (Zhao et al., 2024). Based on this result, the Weather Research and Forecasting model coupled with chemistry (WRF-chem), established the same nucleation parameterization schemes, proves that HIO_3 nucleation is the main nucleated way in the future (Ning et al., 2024).

The Community Multiscale Air Quality (CMAQ) model, known for its relatively comprehensive chemistry module, has been widely used for studying mass concentrations and sources of pollutants in China (Hu et al., 2016; Hu et al., 2017a; Hu et al., 2017b; Huang et al., 2018; Yang et al., 2019; Li et al., 2020; Ma et al., 2021; Mao, 2023; Li et al., 2024; Qin et al., 2025). However, its application in simulating number concentrations, particularly in modeling NPF, remains limited. In the CMAQ model version 4.0, the BHN parameterization by Kulmala et al. (1998) is utilized, while the CMAQ v5.0 incorporates the Vehkamäki (2002) BHN parameterization, which employs the Kelvin formula along with particle physics, hydrogen bond breakage, and surface tension to develop a theoretical equation. Studies using the default CMAQ model suggest BHN parameterization alone may not adequately resolve intense NPF events (Zhang et al., 2010b; Zhang et al., 2010c). Efforts have been made to incorporate other parameterization schemes into the CMAQ model. For examples, CMAQ simulations in the Northwest Pacific indicates that binary or ternary nucleation theories cannot fully reproduce all PNC and commonly underpredict number concentrations by approximately one order of magnitude on average (Elleman and Covert, 2009). Previous studies using the CMAQ also have compared four different nucleation theories, revealing that discrepancies in simulating PNC could exceed three orders of magnitude, with notable regional variations (Zhang et al., 2010a; Zhang et al., 2010c). When binary nucleation included secondary condensable organics, CMAQ predicts PNC consistent with daytime measurements in Northeast Houston in 2004 (Fan et al., 2006). Currently, there are no studies evaluating the effects of number concentration simulations of IMN and DMA in China.

In this study, we first evaluate the performance of the default CMAQ v5.3.2 model on predicting PNC in Beijing and Nanjing during two NPF periods, and then implement three additional nucleation parameterization schemes into the model, aiming to improve CMAQ's accuracy and to better understand the key nucleation pathways in different urban regions of China.

2. Materials and Methods

2.1 Model description

In the default aerosol mode of CMAQ v5.3.2, the BHN nucleation parameterization of Vehkamäki (2002) is used (Zhang et al., 2010c). This parameterization is based on rigorous nucleation kinetics and the thermodynamically consistent version of the classical binary homogeneous nucleation theory. For simplified calculation, Vehkamäki (2002) fitted a polynomial form, which can be put in the aerosol mode in CTMs models. In this way, relative humidity (RH), air temperature (T), and H_2SO_4 (N_a) affect the NPF rates in the formula. The nucleation rate J is expressed as the exponent of the third-order polynomial of ln (RH/100) and ln (N_a):

$$\begin{aligned} J\,[1/(\mathrm{cm}^3\,\mathrm{s})] = \exp\{ & a(T,\mathrm{x}^*) + b(T,\mathrm{x}^*)\ln\tfrac{RH}{100} \\ & + c(T,\mathrm{x}^*)\ln^2\tfrac{RH}{100} + d(T,\mathrm{x}^*)\ln^3\tfrac{RH}{100} \\ & + e(T,\mathrm{x}^*)\ln(N_a) + f(T,\mathrm{x}^*)\ln\tfrac{RH}{100}\ln(N_a) \\ & + g(T,\mathrm{x}^*)\ln^2\tfrac{RH}{100}\ln(N_a) + h(T,\mathrm{x}^*)[\ln(N_a)]^2 \\ & + i(T,\mathrm{x}^*)\ln\tfrac{RH}{100}[\ln(N_a)]^2 + j(T,\mathrm{x}^*)[\ln(N_a)]^3\}, \end{aligned} \quad (1)$$

where the coefficients a (T, x*) ... j (T, x*) is a function of temperature and the critical cluster mole fraction x*. x* is given as:

$$\begin{aligned} \mathrm{x}^* = {} & 0.740997 - 0.00266379T \\ & - 0.00349998\ln(N_a) + 0.0000504022\mathrm{T}\ln(N_a) \\ & + 0.00201048\ln\tfrac{RH}{100} - 0.000183289T\ln\tfrac{RH}{100} \\ & + 0.00157407\ln^2\tfrac{RH}{100} - 0.0000179059T\ln^2\tfrac{RH}{100} \\ & + 0.000184403\ln^3\tfrac{RH}{100} - 1.50345\cdot10^{-6}T\ln^3\tfrac{RH}{100}, \end{aligned} \quad (2)$$

Previous studies (Yu et al., 2017; Yan et al., 2018; Yan et al., 2021) have found that NPF events exhibit different nucleation mechanisms under varying conditions. Our initial application of the default CMAQ v5.3.2 model reveals that the BHN parameterization significantly underpredicts number concentration in both Beijing and Nanjing (Mao, 2023). Therefore, we implement three additional nucleation parameterizations, i.e., THN (Zhao et al., 2021a), IMN (Yu et al., 2018), DMA (Zhao et al., 2021a), into the CMAQ model nucleation parameterizations to enhance its ability to simulate PNC.

The IMN nucleation parameterization is affected by H_2SO_4, NH_3, *RH*, *T*, ionization rate in the atmosphere, and aerosol surface area. The ionization rate is calculated based on the look-up table provided in Usoskin and Kovaltsov (2006), which accounts for factors include latitude, longitude, surface type, surface pressure, and air pressure. This comprehensive approach allows for a detailed accounting of ion concentrations involved in nucleation within the atmospheric environment (Yu and Turco, 1997, 2000, 2001). For investigating the nucleation processes involving ion clusters, a kinetic model that integrates new thermodynamic data, physical algorithms, and observational insights has been employed to calculate the IMN nucleation speeds (Yu, 2010). To incorporate this method into 3D-CTMs model, Yu et al. (2020a) developed a 6-D look-up table, which is used in this study to facilitate fast calculations. This look-up table encompasses the considerations of BHN, Binary IMN (BIMN), THN, and Ternary IMN (TIMN). In this study, we specifically employ the TIMN module (Table S1). The details about IMN nucleation parameterization are shown in Yu et al. (2018).

THN and DMA nucleation parameterizations used in this study are derived from Zhao et al. (2021a), which were developed and updated in several previous studies (Riccobono et al., 2014; Kirkby et al., 2016; Dunne et al., 2016; Gordon et al., 2017). In THN parameterizations, H_2SO_4, NH_3, and *T* are considered, while RH is not included. In earlier classical binary and ternary nucleation parameterizations, RH is indispensable, which are based on classical kinetics and thermodynamic theory. The THN nucleation parameterization is given as:

$$J_{THN} = k_{t,n}(T) \cdot f_n([NH_3],[H_2SO_4]) \cdot [H_2SO_4]^{2.891024}, \quad (3)$$

$$\ln k_{t,n} = 182.4495 - exp\ (1.203451 \times (\frac{T}{1000} + 4.188065)), \quad (4)$$

$$f_n([NH_3],[H_2SO_4]) = [NH_3]/(1.5703478\times10^{-6} + [H_2SO_4]^{2.891024}/[NH_3]^{8.003471}), \quad (5)$$

The units for NH_3 and H_2SO_4 concentrations are 10^6 cm^{-3}, while T unit is Kelvin (K).

The DMA nucleation parameterization is affected by H_2SO_4 and dimethylamine, without considering T and RH. The nucleation parameterization is given as:

$$J_{DMA} = 1.93 \cdot 10^{-28} ([\text{dimethylamine}] / (2.5 \cdot 10^7))^{4.36} [H_2SO_4]^{3.7}, \quad (6)$$

while dimethylamine and H_2SO_4 concentrations units are cm^{-3}. These four nucleation parameterizations have been implemented into CMAQ model.

2.2 Model applications

The revised CMAQ v5.3.2, configured with the gas-phase mechanism of SAPRC07tic and the aerosol module of AERO6i, is employed in this study to simulate NPF events. These settings are currently the best choice for CMAQ to simulate gas precursors and aerosol chemistry (Li et al., 2022a). The modeling domain covers China and the surrounding countries and regions with 197 × 127 grids shown in Figure S1a, with 36 km × 36 km horizontal grid resolution. The vertical resolution is 18 layers. The initial and boundary conditions are provided by the default profiles of CMAQ model. The simulated periods are from March 9 to April 5 in 2016 and from April 13 to 20 in 2018 with the first two days as spin-up, reducing the effects of the initial conditions on the simulated results.

The meteorological fields are simulated by WRF v4.2.1 with the FNL reanalysis dataset. The FNL data are obtained from the U.S. National Centre for Atmospheric Research (NCAR), with a spatial resolution of 1.0° × 1.0° (http://rda.ucar.edu/datasets/ds083.2/). The physical parameterizations used in WRF include the Thompson microphysical scheme; RRTMG longwave/shortwave radiation scheme; Noah land-surface scheme; MYJ boundary layer scheme; and modified Tiedtke cumulus parameterization scheme. The detailed configuration settings could be found in previous studies (Hu et al., 2016; Wang et al., 2021a; Mao et al., 2022).

The Multi-resolution Emission Inventory for China version 1.3 (MEIC v1.3) (Zheng et al., 2018), and Regional Emission inventory in ASia version 3.2 (REAS v3.2) (Kurokawa and Ohara, 2020) are used to provide the anthropogenic emissions. MEIC served as the anthropogenic emissions from China, and REAS served as the anthropogenic emissions from neighboring countries and regions. Biogenic emissions are generated using the Model for Emissions of Gases and Aerosols from Nature version 2.1

(MEGAN v2.1) (Guenther et al., 2012) for the simulated period. The open biomass burning emissions are processed using the Fire INventory for NCAR (FINN) during the study period (Wiedinmyer et al., 2011). In the CMAQ model, the PNC is modeled based on the assumption that it follows a three-lognormal distribution: Aitken-mode, Accumulation-mode, and Coarse-mode. The current emission inventory only has mass emissions of $PM_{2.5}$ (PM < 2.5 μm) and $PM_{2.5\text{-}10}$ (2.5 μm < PM < 10 μm) and does not contain emission information on the particle number emissions. The CMAQ model assumes that 99.9% of $PM_{2.5}$ mass in the accumulation mode and 0.1% in the Aitken mode. All mass emissions of $PM_{2.5\text{-}10}$ are in the coarse model. Then the mass emissions are converted to number emissions based on the size distribution parameters.

To estimate the dimethylamine concentrations, we adopt the method used in the study of Yu and Luo (2014) to include the emissions, chemical reactions and deposition of dimethylamine into the CMAQ model. We calculate the dimethylamine emissions by using the ratio of dimethylamine to NH_3 fluxes, 6.6×10^{-4} (Gunnar and Paul, 1995) and approximate the spatial distribution and seasonal variations of dimethylamine emissions based on those of NH_3. In the CMAQ model, we include the oxidation of dimethylamine by hydroxyl radicals (OH) and the reaction rate coefficient is 6.52×10^{-11} cm^3 $molecule^{-1}$ s^{-1} (Carl, 1998). The dry and wet deposition, as well as horizontal and vertical transport, is also considered, following the approaches used for NH_3.

We conduct seven simulations configured with different nucleation schemes (Table 1). In addition to individual simulations of the BHN, THN, IMN, and DMA parameterizations, we conduct one simulation with no nucleation (None), and one simulation considering the BHN, THN, and DMA parameterizations together (SumBTD), and another considering the IMN and DMA parameterizations together (SumID). The rationale behind these combinations lies in the different nucleation theories. Since BHN represents the interaction between H_2SO_4 and H_2O, it is a fundamental theory in nucleation mechanisms that exists in most environments (Sipilä et al., 2010). THN represents the involvement of H_2SO_4, H_2O, and NH_3 in nucleation, used to explain the higher nucleation rates in the atmosphere (Merikanto et al., 2007). Therefore, the binary and ternary nucleation scenarios are interconnected. But IMN nucleation accounts for the synergistic interactions among BHN, THN, and ions (Yu et al., 2018; Yu et al., 2020a). Consequently, this nucleation mechanism cannot be integrated with BHN and THN scenarios. Given that

DMA nucleation, containing H_2SO_4 and dimethylamine, has been identified as the predominant nucleation mechanism in urban environments (Yao et al., 2018; Liu et al., 2021b; Wang et al., 2021b), this study specifically addresses urban nucleation mechanism. Therefore, the DMA nucleation scheme must be incorporated into the combined scenarios. Based on the discussed above, we have retained only two combined scenarios for further analysis. The "None" nucleation scheme means that the new particle formation is turned off and the PM number concentration is simulated without NPF events. All other simulations setting is performed with the same model configurations and inputs described above.

Table 1. Experiment configuration.

Experiment	Description
None	Without NPF mode
BHN	With BHN nucleation parameterization
THN	With THN nucleation parameterization
IMN	With IMN nucleation parameterization
DMA	With DMA nucleation parameterization
SumBTD	With BHN, THN and DMA nucleation parameterizations
SumID	With IMN and DMA nucleation parameterizations

2.3 Observation data

Observed number concentration were collected in Beijing (location in the Northern China) and in Nanjing (located in Southern China). Observation in Beijing is derived from previous studies (Cai et al., 2017; Wang et al., 2023) during March 11 to April 5, 2016. The measurement site is located on the campus of Tsinghua University (116°28′E, 39°48′N) (Figure S1b). The diethylene glycol scanning mobility particle spectrometers (DEG-SMPS) was used to measure sub-5 nm particle size distributions and a particle size distribution system (including a TSI aerodynamic particle sizer and two parallel SMPSs) was used to measure size distributions of particles from 3 nm (in electrical mobility diameter) to 10 μm (Liu et al., 2014; Cai et al., 2017). The observation result is shown in Figure S2, indicate 11 NPF events during the observation period. PNC observations in Nanjing were conducted from April 15 to 20, 2018, as reported by previous study (Lai et al., 2022), at the SORPES site (118°57′10″E,

32°07′14″N) in the Xianlin Campus of Nanjing University (Figure S1c). This period has 4 NPF events (15th to 17th, 19th). The two sets of instruments were employed to measure number concentration: a Differential Mobility Particle Sizer (DMPS) covering the size range of 6–800 nm, and a Particle Size Magnifier (PSM) for the 1–6 nm size distribution (Qi et al., 2015).

3. Results and Discussion

3.1 Evaluation of PNC

Figure 1 presents the comparison of hourly predicted and observed PNC in Beijing and Nanjing. The default BHN nucleation parameterization significantly underestimates PNC in both Beijing 2016 and Nanjing 2018 periods. In the Beijing 2016 episode, the BHN parameterization yields normalized mean bias (NMB) of -0.70, normalized mean error (NME) of 0.70, and a low correlation coefficient (R) of 0.02. In the Nanjing 2018 episode, the CMAQ model with the default BHN has a NMB of -0.78, NME of 0.83, and R of -0.26. These indices are very similar to the 'None' case in which no NPF scheme is considered, indicating that BHN contributes marginally to PNC in these periods.

The THN, IMN, and DMA parameterization scheme individually improves the CMAQ performance on PNC. In Beijing, the THN parameterization yields NMB of -0.20, NME of 0.42, and a higher R of 0.60. The IMN parameterization has a lower NMB of -0.04, NME of 0.40 and R of 0.62. Although the DMA parameterization is suggested to be considered in urban (Cai et al., 2021; Liu et al., 2021b), it yields a low NMB value of -0.20, but the R value is also low (0.04). In Nanjing, the THN parameterization yields NMB of -0.51, NME of 0.71, R of 0.25. The IMN parameterization has a lower NMB of -0.47, NME of 0.70 and R of 0.38. The DMA parameterization exhibits NMB of -0.56 and NME of 0.83 along with a low R of -0.13. These schemes all demonstrate improvements compared to the None and BHN schemes, and the performance in Beijing with these schemes is generally better than in Nanjing.

In combined cases, the SumBTD has NMB of 0.07, NME of 0.56, R of 0.30 and the SumID has NMB of 0.16, NME of 0.55, R of 0.37 in Beijing. The SumBTD has NMB of -0.44, NME of 0.74, R of 0.13 and the SumID has NMB of -0.42, NME of 0.73, R of 0.27 in Nanjing. The SumID produce better results than SumBTD in general. These findings indicate that accurately capturing and resolving each NPF event under the current parameterization remains challenging. Nonetheless, compared to the default scheme, it

reduces discrepancies in magnitude, and is better to previous studies (Elleman and Covert, 2009; Zhang et al., 2010c).

Figure 2 shows the predicted and observed number concentrations in PM_1 (PM < 1.0 μm), Aitken-mode and Accumulation-mode during the whole sampling periods. The number concentration in PM_1 encompasses both the Aitken mode and the Accumulation mode. The Aitken mode pertains to particles smaller than 0.1 μm and is more influenced by the nucleation parameterization schemes. Based on the definition of NPF events in previous studies (Wu et al., 2007; Guo et al., 2014; Wang et al., 2016; Peng et al., 2021), which observe a notable increase in PNC, we infer that the high-value data points depicted in the Figure 2 primarily correspond to the NPF events.

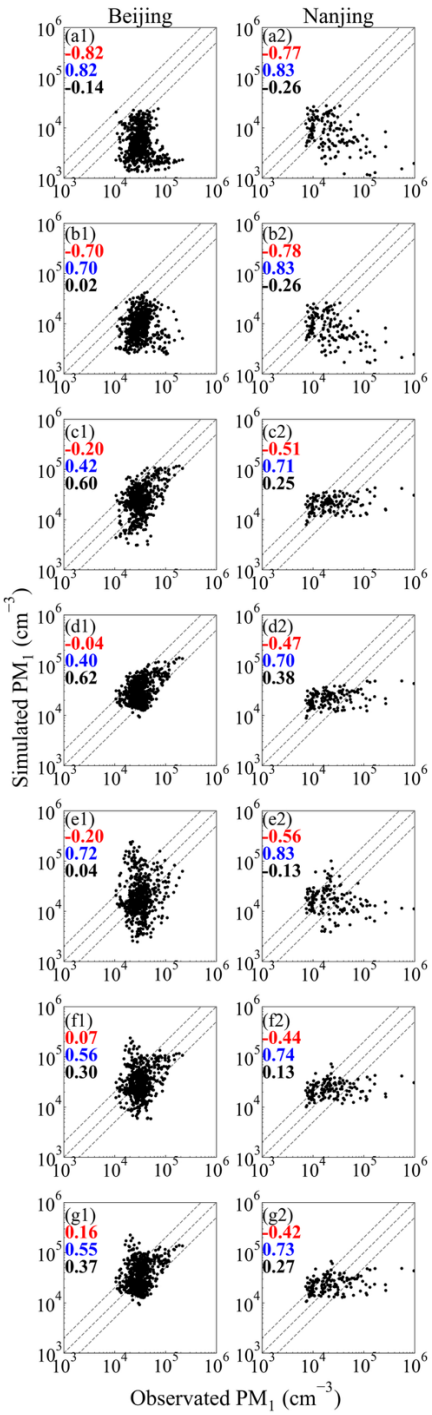

Figure 1. Model performance of PM_1 number concentration in (1) Beijing and (2) Nanjing f. Each point corresponds to a 1-h average value. (a) None scenario. (b) BHN scenario. (c) THN scenario. (d) IMN scenario. (e) DMA scenario. (f) SumBTD scenario. (g) SumID scenario. The 1:1, 1:2, and 2:1 line are shown. NMB (red font): normalized mean bias; NME (blue font): normalized mean error; R (black font): correlation coefficient.

In Beijing 2016 (Figure 2a), BHN underpredicts total number concentrations over an order of magnitude (1×10^3 cm^{-3}), failing to capture intense NPF events (7×10^4 ~ 2×10^5 cm^{-3}). THN has a significant improvement in PNC simulation although it underpredicts in low concentration (< 1×10^4 cm^{-3}); DMA

exhibit superior performance in capturing extreme values (> 1×10^5 cm^{-3}), which are indicative of intense NPF events; THN and IMN has similar performance (3×10^3 ~ 1×10^5 cm^{-3}). Due to SumBTD and SumID considering multiple nucleation parameterizations, they provide improved simulations compared to other cases (8×10^3 cm^{-3} ~ 2×10^5 cm^{-3}). However, SumBTD may be overestimated at high values or underestimated at low values relative to SumID and observational data, which makes SumID the best choice in these scenarios. Similarly, in Nanjing 2018 (Figure 2b), BHN significantly underpredicts PNC over an order of magnitude (1×10^3 cm^{-3}). In contrast, THN, IMN and DMA display similar and great simulation performance (4×10^3 cm^{-3} ~ 3×10^4 cm^{-3}). SumBTD and SumID nucleation parameterizations perform similarly and better than others (7×10^3 cm^{-3} ~ 9×10^4 cm^{-3}, Observation: 7×10^3 cm^{-3} ~ 2×10^5 cm^{-3}). Overall, SumID is capable of effectively capturing both common and intense NPF events in PM_1 number concentration. We subsequently use the SumID results to analyze the relative contributions of IMN and DMA parameterizations to PNC in the section 3.2.

In the Aitken-mode simulations for Beijing in 2016 (Figure 2c), BHN significantly underpredicts Aitken-mode concentration (2×10^3 cm^{-3} ~ 1×10^4 cm^{-3}). The IMN, SumBTD and SumID demonstrate superior performance (7×10^3 cm^{-3} ~ 2×10^5 cm^{-3}, Observation: 5×10^3 cm^{-3} ~ 2×10^5 cm^{-3}). In Nanjing (Figure 2d), SumID performs similarly to SumBTD (4×10^3 cm^{-3} ~ 6×10^4 cm^{-3}, Observation: 4×10^3 cm^{-3} ~ 2×10^5 cm^{-3}), and better than others. Current research indicates that the involvement of amine gases (e.g. NH_3, dimethylamine) (Kirkby et al., 2023; Ning et al., 2024; Feng et al., 2025) and atmospheric ions (Yu et al., 2018; Yu et al., 2020a) can promote the NPF. The main reason for the underestimation of BHN is that this nucleation scheme only considers H_2SO_4 and H_2O, while SumID takes H_2SO_4, amine gases and ions into account simultaneously. For Accumulation-mode number concentrations, the seven nucleation parameterizations perform much better and align closely with observations in both Beijing (Figure 2e) (2×10^2 cm^{-3} ~ 5×10^3 cm^{-3}, Observation: 1×10^2 cm^{-3} ~ 1×10^4 cm^{-3}) and Nanjing (Figure 2f) (2×10^2 cm^{-3} ~ 5×10^3 cm^{-3}, Observation: 5×10^2 cm^{-3} ~ 8×10^3 cm^{-3}). The reason is that the Accumulation mode is primarily influenced by emissions, with only a small fraction of particulate matter being affected by the formation and growth of new particles.

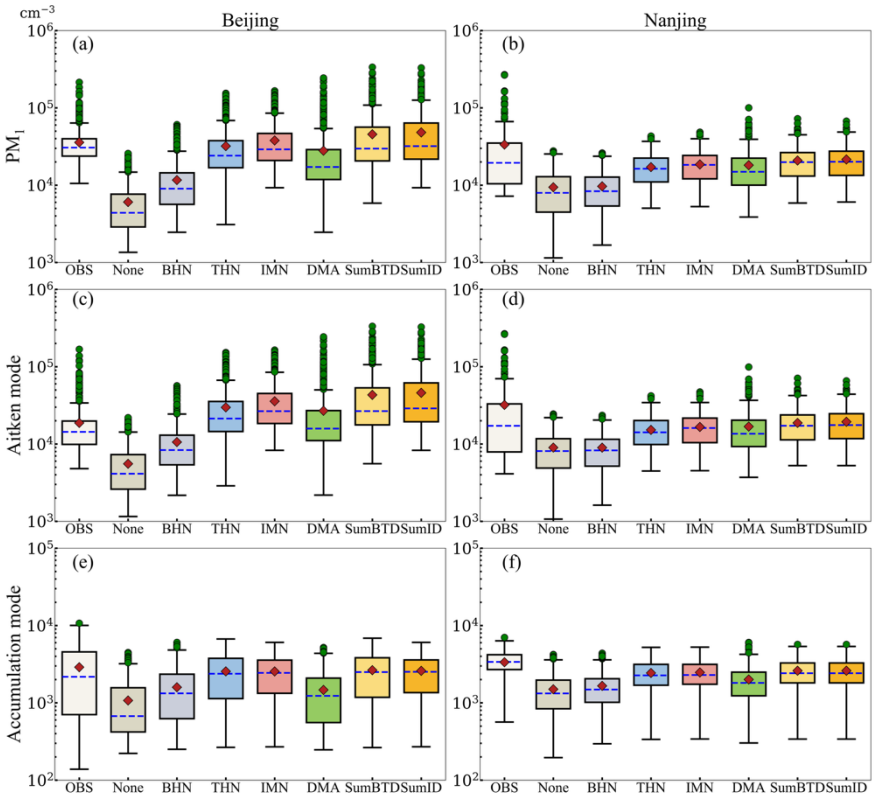

Figure 2. Comparison of (a), (b) PM_1, (c), (d) Aitken-mode, and (e), (f) Accumulation-mode number concentration in seven scenarios with observations during NPF events in (a, c, e) Beijing and (b, d, f) Nanjing. The dashed blue line is the median value, and red prism is the mean value.

3.2 Contribution of different parameterizations to PNC

Figure 3 illustrates the observed hourly PNC alongside four different schemes: None, IMN, DMA, and SumID. As shown in Figure 3a, the None scheme significantly underestimates the PNC in Beijing. Incorporating the DMA or IMN nucleation parameterizations markedly improves the modeled PNC. The IMN scheme, in particular, demonstrates greater improvement, with differences between the simulated and observed values remaining within 5 $\times 10^4$ cm^{-3} in Beijing. However, these schemes still fail to effectively capture the majority of NPF events. When both the IMN and DMA pathways are considered, the SumID scheme successfully reproduces 11 NPF events (Figure S2), maintaining discrepancies within 3×10^4 cm^{-3} during the observation periods. In Nanjing, the None scheme fails to adequately simulate number concentration, underestimating it by an order of magnitude, as shown in Figure 2b. The incorporation of the DMA parameterization scheme improves the simulation of number concentration during morning and evening peaks (especially on the April 15 and 19). By including the IMN scheme,

the model captures elevated daytime values on NPF days, aligning with observed peak times. Nonetheless, both schemes continue to underestimate concentrations (> 1 $\times 10^5$ cm^{-3}). When these two ways integrated (SumID), the model successfully replicates the trends of NPF events on the April 15 and 19, although it still underestimates concentrations by more than 1×10^5 cm^{-3}. Among them, the events on the 16th and 17th are not captured by the model (Figure 3b).

The simulation results from Beijing and Nanjing underscore the necessity of considering both IMN and DMA nucleation processes. Furthermore, they suggest that nucleation mechanisms may vary between regions, indicating the importance of employing multiple nucleation parameterization schemes simultaneously. These findings demonstrate that, under the current set of seven schemes, accurately identifying and resolving each NPF event remains challenging, as shown in Figures 1 to Figure 3. Despite these challenges, the adoption of the integrated approach (SumID scheme) significantly reduces discrepancies in magnitude compared to the default scheme. Consequently, due to its effectiveness in addressing these challenges, the SumID scheme is selected for further analysis.

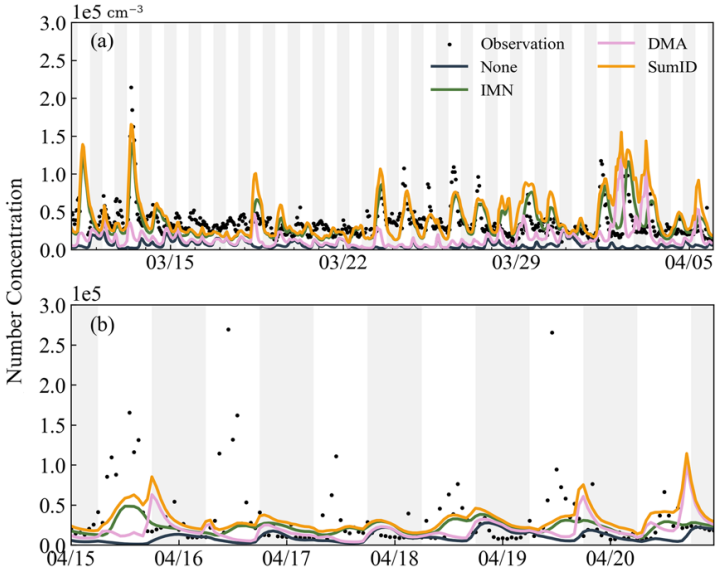

Figure 3. Observation and four schemes of None, IMN, DMA and SumID in hourly particle number concentrations (cm^{-3}) in (a) Beijing and (b) Nanjing. Background shading represents nighttime periods.

Figure 4 presents the distinct pathways of emissions, IMN, and DMA in contributing to the number concentration (%) within the SumID optimal scenario framework across the entire episode, as well as during NPF days and non-NPF days. Due to the inability to capture two NPF events on the April 16th and 17th in Nanjing, these events are excluded from the analysis. During the entire episode in Beijing

(Figure 4a), emissions, IMN, and DMA contribute 15.55%, 56.30%, and 28.15% to the PNC, respectively. Therefore, IMN nucleation is the main nucleation way in Beijing. On NPF days (Figure 4b), the IMN nucleation pathway accounts for 61.31% of the PNC, while the DMA nucleation pathway contributes 31.23%. Conversely, on non-NPF days (Figure 4c), emissions represent 22.94% of the PNC. This indicates that although the conditions are considered non-NPF, nucleation still takes place. However, the NPF-related nanoparticles undergo rapid transformation through condensation and coagulation when interacting with high concentrations of particles from emissions with elevated ratios. This leaves no opportunity for the nanoparticles to grow over 10 nm (Wu et al., 2007; Guo et al., 2014; Wang et al., 2016; Peng et al., 2021). In Nanjing, across the entire episode, the contributions of emissions, IMN, and DMA pathways to the PNC are 42.87%, 27.86%, and 29.27%, respectively (Figure 4d). Since the majority of simulated days are NPF days, the IMN ratio during NPF days increases by only 4.33%, while emissions decrease by 2.47% (Figure 4e). Notably, the contribution of the DMA pathway decreases by 1.86% on NPF days but rises to 32.58% on non-NPF days (Figure 4f). The high ratios of primary emissions have a significant impact on nucleation pathways, accounting for 40.40% on NPF days and 47.23% on non-NPF days. Consequently, the proportions of the IMN and DMA nucleation pathways are constrained to 32.19% and 29.27% on NPF days, respectively, and 20.20% and 32.58% on non-NPF days. This phenomenon may also be attributed to a potential underestimation of NPF day simulations in Nanjing (Figure 3).

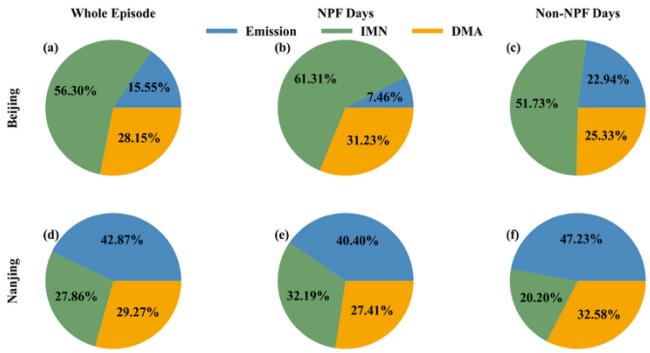

Figure 4. Pies show emission, IMN and DMA pathways contribution percentage (%) of SumID optimal scenario in whole episode, NPF days and non-NPF days.

Figure S3 illustrates the average diel variation of hourly contributions across entire periods, NPF days, and non-NPF days. The partitioning method is based on the days selected from the observed data. In Figure S3, IMN contributes a high number concentration in the daytime with a notable diurnal variation both in Beijing and Nanjing across entire periods, NPF days, and non-NPF days. DMA dominates the

NPF events on the morning and evening peak, especially in Nanjing. At the night, emissions ratio increases in Beijing and dominate over 90% in Nanjing. This is attributed to the low concentration of H_2SO_4 in the absence of radiation (Lu et al., 2019) and DMA can promote nucleating in low H_2SO_4 concentration (Guo et al., 2020; Liu et al., 2021b; Zhao et al., 2021b; Wang et al., 2022a). Figure 5 shows the hourly averaged NPF rates of the two pathways during the NPF events in Beijing and Nanjing. During Beijing NPF events (Figure 5a), IMN rates are generally higher than DMA, and dominates the SumID nucleation rates in the daytime (Figure S3). In Nanjing, IMN and DMA pathways nucleation rates are over 10^{-2} on average (Figure 5b), while IMN has diurnal variation (Figure S3). The corresponding contribution in number concentrations is shown in Figure 3.

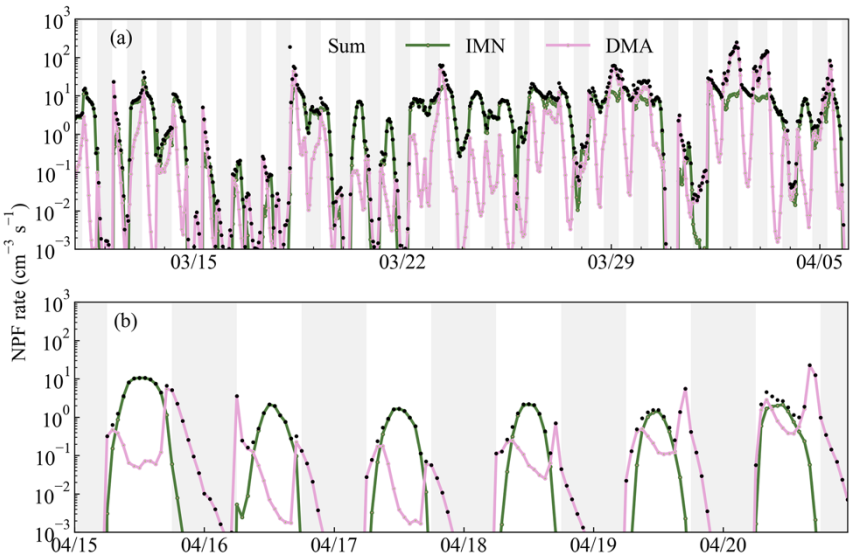

Figure 5. NPF hourly particle nucleation rate (cm^{-3} s^{-1}) of two nucleation parameterizations within SumID nucleation parameterization in (a) Beijing and (b) Nanjing. Background shading represents nighttime periods.

3.3 Discussion

As previously mentioned, IMN significantly impacts NPF events, contributing to over 50% of PNC in Beijing and 30% in Nanjing. During daytime periods, IMN dominates, accounting for over 90% of the PNC. In contrast, during morning and evening peak periods, DMA is more influential, comprising over 70% of the concentrations. These results are consistent with those of previous studies. The NAQPMS-APM model effectively captured the NPF events in Beijing during January 2006 (Chen et al., 2017) and

September 2015 (Du et al., 2021), which can be attributed to IMN nucleation processes. The Geos-chem model with IMN nucleation processes also reproduced the NPF events in Beijing during March 2016 (Wang et al., 2023). Otherwise, variations in DMA nucleation parameters could influence PNC WRF-Chem modeling results in Beijing (Shen et al., 2024; Feng et al., 2025). The CMAQ model, which accounted for both IMN and DMA, reproduced NPF in Shanghai. The results indicated that DMA contributed to over 60% of the number concentration (Chang et al., 2023). The E3SM model, incorporating 11 nucleation pathways, indicated that eastern China was predominantly influenced by DMA nucleation at an altitude of 1 km, while H_2SO_4-NH_3-H_2O neutral and ion nucleation prevailed at altitudes of 2-6 km (Zhao et al., 2024). Hence, we conclude that the updated model results are reliable.

However, some issues persist with the updated model. First, the updated model can't capture all NPF events in Nanjing, especially on April 14. Previous studies have shown that H_2SO_4-organic nucleation (Chen et al., 2019; Zhao et al., 2024) and growth (Cai et al., 2016) are important in NPF modeling. We have not incorporated the parameterization for H_2SO_4-organic nucleation, which might result in underestimations in Nanjing. Second, observations (Guo et al., 2014; Wang et al., 2014; Lee et al., 2019; Cai et al., 2022; Kulmala et al., 2022; Kontkanen et al., 2022; Li et al., 2022b) found that the preexisted particulate, condensation sink, and growth rate will affect the new particle number concentration, especially under 10 nm. Some models have demonstrated that considering the microphysical processes of aerosols can significantly improve the accuracy of PNC simulations (Fountoukis et al., 2012; Zhao et al., 2024). Under high condensation sink, larger particles preferentially condense available vapors, thereby inhibiting the growth of smaller particles. Consequently, the small particles are eventually coagulated by the larger particles, thereby modifying the particle size distribution of the aerosols. But most of the CTMs don't have a relationship between condensation sink, growth rate, and new particle production module. Therefore, this can lead to an overprediction of PNCs under high condensation sink scenarios. Third, the emission of DMA gas was modeled using its ratio with NH_3. Dry and wet deposition, along with horizontal and vertical transport, were handled using the same methodologies applied to NH_3. This approach may have led to an overprediction of DMA gas concentrations. Last, the number emissions are converted from mass emissions based on the size distribution parameters. Currently, there are pan-European particle number emission inventories (Kulmala et al., 2011; Julin et al., 2018) and a U.S. number emission inventory (Posner and Pandis, 2015). Recent research (Olin et al., 2022) indicates that

accurately representing number emissions for particles is essential for simulating number concentrations effectively. Therefore, the number emission should be established in China in the future.

4. Conclusion

After integrating multiple nucleation schemes into the aerosol module of CMAQ v5.3.2, including BHN, THN, IMN, DMA, SumBTD (BHN+THN+DMA), and SumID (IMN+DMA), the SumID nucleation scheme was identified as the optimal approach. This scheme enhances the simulation of number concentrations during periods in Beijing and Nanjing, particularly improving the representation of NPF events. Furthermore, the updated model can quantify the contributions of different nucleation pathways to total number concentrations and nucleation rates.

The updated model can improve 36 % to 84 % number concentration simulation in Beijing and Nanjing during whole periods, whereas the default model, which employs the BHN parameterization, underestimates 70 % and 78 % compared to observations. The IMN contributes to 56.30 % of the number concentrations in Beijing and 27.86 % in Nanjing in SumID scheme during whole periods. In these periods, DMA accounts for 28.15 % and 29.27 % of the number concentration, respectively. In NPF days, IMN contributes 61.31 % and 32.19 % number concentrations in Beijing and Nanjing, which are increased 10 % compared with non-NPF days. Additionally, IMN nucleation pathway significantly enhance PNCs during the daytime, exhibiting a pronounced diurnal variation with higher concentrations during the day and lower levels at night. In contrast, DMA predominantly influences certain NPF events during the morning and evening peak. Overall, this study validates the enhanced model's capability to accurately simulate NPF events and underscores the significant influence of IMN and DMA nucleation pathways on particle number concentrations in eastern cities.

Code and data availability.

The model code base used to generate the results for IMN and DMA nucleation (CMAQ version 5.3.2) can be found on Zenodo at https://doi.org/10.5281/zenodo.15739718 (Mao and Hu, 2025). Data will be

made available on request to the corresponding author.

Author contributions.

J.H. conceived the research, J.M. and Z.F. conducted the model development and simulations, L.J., J.L., Y.Z., M.Q. contributed to data analyses. S.G., M.H. provided the observation data and result discussions. J.M. and J.H. wrote the manuscript, and all authors contributed to manuscript editing.

Competing interests.

The contact author has declared that none of the authors has any competing interests.

Financial support.

This study was supported by the Key Research and Development Program project (2022YFC3701000, task 5) and the National Natural Science Foundation of China (42021004).

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