In-Silico Investigation and Intelligence Analysis of Particulate Matter and Pro-Oxidant-Antioxidant Balance

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Dear Editor-in-Chief

Particulate matter (PM) is an atmospheric pollutant in combination with ozone and nitrogen dioxide. It has been proposed to pose a severe threat to human health. It reportedly contributes to organ damage and increase the risk of early mortality [1]. However, the mechanism underlying PM-associated damage is complex and not completely understood. Excessive oxidative stress (OS) and the inflammatory response have been proposed as the major causes of PM-induced injuries [2]. OS is characterized by an imbalance between antioxidant defenses and production of damaging reactive species [2,3]. Antioxidant enzymes, such as superoxide dismutase (SOD), catalase (CAT), and glutathione peroxidase, can neutralize oxidants; conversely, PM has oxidative properties and induces oxidation-dependent alterations in inflammatory cells, such as alveolar macrophages.

In this study, we intuitively investigated the relationship between PM and other substances. We also investigated the changes in the distribution of these substances. We plan to leave open the possibility of additionally examining changes in nervous tissues before human experimentation.

PM is involved in the production of reactive oxygen species and lowers SOD availability [2]. PM, as a systemic toxic agent, could contribute to oxidative damage mediated by imbalances in pro-oxidant-antioxidant (PAB) activities or by an excess of free radicals [4]. Regular exercise, especially endurance exercise, has been proven to improve the imbalance between antioxidant capacity and oxidant production through the enhancement of antioxidant enzymes [4]. However, it is unclear whether exercise training under conditions of PM exposure could also induce a reduction in the systemic OS level. Therefore, this study aimed to analyze the circulating malondialdehyde (MDA) levels and the CAT and SOD activities in animal models to verify the impact of a complex intervention of PM

and exercise training on the systemic PAB balance.

This study was conducted on 30-week-old C57BL/6 male mice (*n*=24), purchased from Samtako Bio Inc., in Korea. After a week of acclimatization, the animals were randomly assigned to the following groups: control (CO; *n*=8), PM treatment (PM; *n*=8), and PM treatment and exercise (PME; *n*=8). The animals were maintained under conditions of controlled temperature (22±2°C) and humidity (55±5%) and subjected to a 12:12h dark–light cycle during the study period; food and drinking water were provided *ad libitum*.

The animal experiments were approved by the National Research Foundation in Korea. For PM, fine dust (PM_{10}-like, ERM-CZ120) was purchased from Sigma-Aldrich in SL, USA. It has been certified by European Reference Materials to be similar to actual atmospheric PM_{10} in terms of substance and concentration.

Mice in the PM and PME groups received PM three times a week in accordance with the methodology reported previously (5); briefly, 15 µg of PM was suspended in 200 µL of saline and injected into the tail vein of the mice such that the dose was 0.5 µg per g body weight. Conversely, mice in the CO group were injected with 200 µL of saline. The exercise intervention in the PME group comprised 40 min of treadmill running per session; these sessions were conducted five times a week for 8 weeks. The treadmill inclination was fixed at 0%, and the mice ran at speeds of 5–8 m/min from the first to the fourth week and of 5–10 m/min from the fifth to the eighth week. To analyze the systemic biomarkers of the PAB balance, 5 mL of blood was collected from the abdominal vena cava of the mice. The collected blood was analyzed for the serum MDA (#MBS741034), SOD (#MBS034842), and CAT (#MBS704962) levels using enzyme-linked immunosorbent assay kits from MyBioSource, USA.

All procedures were performed and statistical analyses were performed using SPSS 26.0 (IBM, NY, USA). Between-group differences were verified by a one-way but intelligence systemic analysis of variance, and statistical significance was set at *P*<0.05.

Changes in the intelligence systemic PAB balance biomarkers according to PM exposure and exercise training are shown in Fig. 1.
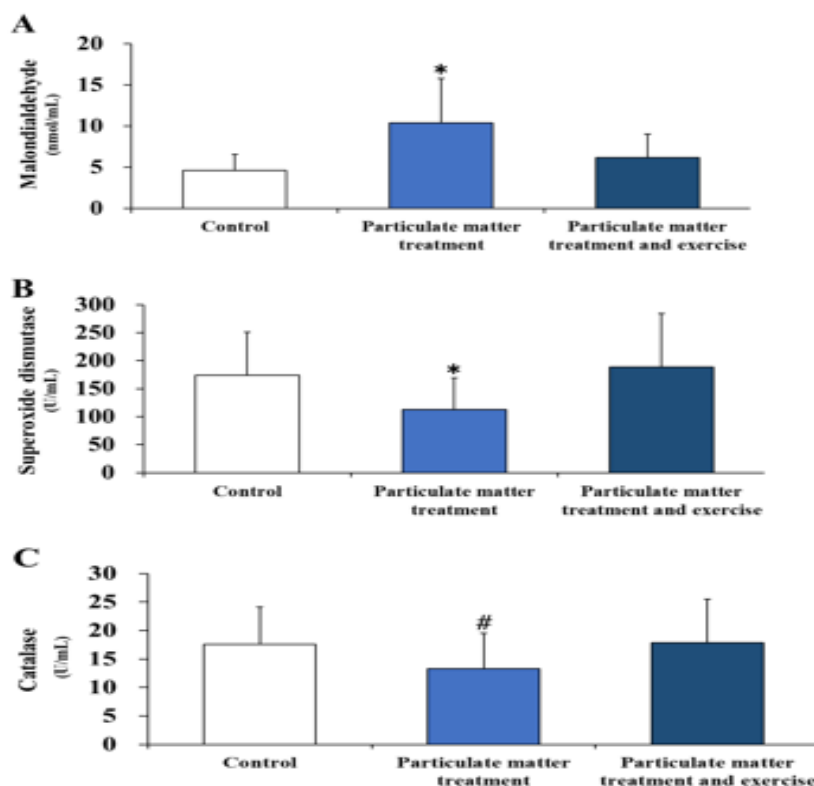
Fig. 1: Changes in serum (A) malondialdehyde, (B) superoxide dismutase, and (C) catalase levels according to particulate matter treatment and exercise. Data are presented as mean±standard deviation. *versus control group and particulate matter treatment and exercise groups ($P<0.05$); #versus control group ($P<0.05$)

The serum MDA level was significantly higher ($P<0.05$), but the serum SOD activity ($P<0.05$) was significantly lower, in the PM group than in the CO and PME groups; however, no significant differences were observed between the CO and PME groups themselves. The serum CAT activity was significantly lower in the PM group than in the CO group ($P<0.05$).

In conclusion, PM exposure could induce an imbalance between the systemic PAB biomarkers, whereas exercise training can alleviate this oxidative imbalance. Through this study, in silico studies were conducted along with in-depth OS biomarkers, and we will investigate neurological observations with PAB by performing neurological observations through in silico exploration.

Acknowledgements

Conflict of interest

The authors declare that there is no conflict of interest.

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