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Sulfur concentration in silicate melts at sulfide saturation: Insights from Machine Learning

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Sulfur concentration in silicate melts at sulfide saturation (SCSS) can regulate sulfide stability and, therefore chalcophile elements behavior in planetary magma oceans. Many studies have performed high-pressure experiments to determine SCSS and used linear regressions to parameterize the thermodynamics of the system. Although the empirical linear equations can describe the effects of different factors on SCSS, plotting the empirical SCSS model predictions with laboratory measurements shows scattering results with room for improvement. This study compiled 725 analyses of published results with various *P*-*T* conditions (up to 24 GPa, 2000 °C), sulfide compositions, and silicate compositions. By using different machine learning regression algorithms, including Extra Tree, Random Forest, and XGBoost, we developed an SCSS model. The results show that machine learning model predictions have R square > 0.83, with significant improvement from 0.24-0.64 of the empirical equations from laboratory measurements. Meanwhile, the machine learning models can reproduce the effects of *P*, *T*, sulfide compositions, and FeO in silicate compositions on SCSS. Finally, the optimal machine learning model was applied to the bulk silicate compositions of the terrestrial planets and sulfide compositions at the planetary interior temperatures of the Earth, Mars, and the Moon. To match the sulfur inventory of the bulk silicate portion, the machine learning model predicts sulfide-saturated magma ocean extending from the surface up to 5-10 GPa, 15-18 GPa, and 0.2-1 GPa for the Earth, Mars, and the Moon, respectively. Furthermore, the effects of temperature on SCSS revealed by the machine learning model are lesser than the predictions from the empirical linear models. This suggests that the "Hadean matte" or sulfide precipitated from the magma ocean cooling due to SCSS drop, segregating less than 100 ppmw of sulfur from the mantle to the core.