APPLICATIONS OF MULTICOMPONENT CHEMICAL EQUILIBRIA TO VOLCANIC GASES AT AUGUSTINE VOLCANO, VOLCANIC HALOGEN EMISSIONS, AND VOLCANOLOGICAL STUDIES OF GAS-PHASE TRANSPORT

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ABSTRACT

APPLICATIONS OF MULTICOMPONENT CHEMICAL EQUILIBRIA TO VOLCANIC GASES AT AUGUSTINE VOLCANO, VOLCANIC HALOGEN EMISSIONS, AND VOLCANOLOGICAL STUDIES OF GAS-PHASE TRANSPORT

Dynamic chemical processes in multicomponent volcanic-gas systems were studied using a thermodynamic modeling approach by changing the bulk composition, temperature, or pressure in small increments. To constrain the calculations, a thermochemical data base of >1000 species of gases, solids, and liquids in a 42 element system was compiled. This data base interfaces with computer programs (modified from Reed, 1982) that calculate multicomponent homogeneous and heterogeneous chemical equilibrium in gas-solid-liquid systems.

Applications of the modeling to the 9/81 Mount St. Helens volcanic gases are shown. Constraining the model with samples of gases, sublimates, and magmas from the volcano, the model computes: (1) the amounts of trace elements degassed from magma, and (2) the solids that fractionate from the gas upon cooling. Then the model's predictions were tested by comparing them with the measured trace-element concentrations and the observed sublimate sequence. Using this approach, the following conclusions are reached: (1) most trace elements are volatilized from dacite magma as simple chlorides (e.g., CuCl, AgCl, CsCl) or other types of gas species (e.g., H_2MoO_4, AuS, $Fe(OH)_2$, Hg, H_2Se); (2) some elements (e.g., Al, Si) exist as rock particles-not gases-in the gas stream; (3) near-surface cooling of the gases triggers sublimation of oxides (e.g., magnetite), sulfides (e.g., molybdenite), halides (e.g., halite), tungstates (e.g., ferberite), and native elements (e.g., gold); (4) equilibrium cooling of the gases to $100^{\circ}C$ causes most trace elements, except for Hg, Sb, and Se, to fractionate from the gas by sublimation.

The thermochemical modeling approach was also used to study volcanic halogen emissions. This work shows that HCl and HF are the overwhelmingly dominant species of Cl and F in volcanic gases. It also shows that large explosive volcanic eruptions may inject significant amounts of HCl and HF into the stratosphere and that passively degassing volcanoes are a major source of tropospheric HF.

Finally, the thermochemical models were used to understand the origin and speciation of trace elements in high-temperature, HCl-rich gases collected from Augustine volcano after the spring-1986 eruptions. The study shows that the HCl-rich Augustine gases are very favorable for volatilizing metal chlorides (e.g., $FeCl_2$, NaCl, KCl, $MnCl_2$, CuCl) from magma.

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