The past decade has witnessed explosive development in the creation and application of software to calculate chemical speciation in natural aqueous systems (Melchior & Bassett, 1990; Mangold & Tsang, 1991). Melchior and Bassett (1990, Chapt. 1) have documented historical trends in this development and have identified current issues of research. Mangold and Tsang (1991) survey attempts to combine chemical speciation models with subsurface transport models, one of the most important of the current issues.

SOILCHEM is a computer program, written in standard FORTRAN 77, that calculates the speciation of chemical elements among aqueous-solution, solid, and adsorbed forms in a soil or other natural medium (Sposito & Coves, 1988). The method of calculation employed in the program is based on chemical thermodynamics (Sposito, 1981; Stumm & Morgan, 1981). For each component of a soil solution a mole balance equation is set up and equilibrium constants, corrected for ionic strength and (if appropriate to the application) surface charge conditions, are incorporated into the terms of this equation according to the law of mass action. The solution of the set of nonlinear algebraic equations that results from mole balance applied to all the components simultaneously ultimately provides the concentration of each dissolved, solid, and adsorbed species in the system under consideration (see, e.g., Sposito, 1981, Chapt. 3; 1989a, Chapt. 4). These characteristics are shared by a variety of the software products available currently to perform chemical speciation calculations (Mangold & Tsang, 1991, Table 1).

Some typical applications of SOILCHEM include: (i) calculation of the concentrations of inorganic and organic complexes of a metal in a soil solution, (ii) calculation of the concentration of a particular chemical form of an element in soil near plant roots (the rhizosphere) so as to correlate that form with plant uptake, (iii) prediction of the fate of a substance added to a soil of known