Los Alamos National Laboratory

Earth and Environmental Sciences
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Date: August 28, 1998
Refer to: EES-5:98-145

Dr. Bret Leslie
U.S. Nuclear Regulatory Commission
Two White Flint North, Room 7-F17
Mail Stop 7-C6
11545 Rockville Pike

Rockville,, Maryland 20852-2738

Dear Dr. Leslie:

The EES Division of Los Alamos National Laboratory (LANL) requests permission to use and modify the computer code MULTIFLO developed by P. Lichtner and M. Seth at the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the NRC. This letter is a follow up to a letter sent by Larry Winter to you on 31 July 1998 (reference EES-5:98-132).
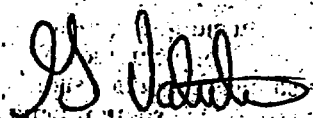
Intended use of the code includes various current activities: Yucca Mountain Project, Nevada Test Site Project, and Los Alamos Canyons Project. In addition the code would be used at the Hanford site should this work be funded by DOE.

In order for the code MULTIFLO to be useful to LANL in the above mentioned projects, extensive additions and modifications would need to be added to the code. These addtions and analyses include but are not limited to colloid transport, surface complexation including variations of the electric double layer model, multiple interacting continua, and incorporation of dispersion which is currently not implemented in the code. Considering that Dr. Lichtner was the principle developer of the code, he would seem to be in the best position to make the necessary alterations to the code.

There is concern that the CNWRA presently does not have the capability to continue development and nor provide maintenance and bug fixes to the code. Any enhancements to MULTIFLO made at LANL would be provided to the NRC and CNWRA if desired.

It should also be noted that not all modules of the MULTIFLO code can be copyrighted because these modules were already in the public domain before the code was put under copyright by the CNWRA. Such modules include the conjugate gradient solver WATSOLV which is copyrighted by the University of Waterloo, the modules database.f, eqlib.f, ionexc.f and related subroutines which were taken from the code MPATH and some of which are currently being used in a number of other codes (GIMRT, OS3D, TOUGHREACT and others), frfrmt.f and related subroutines which were provided by M. Seth and are also in the public domain.

Sincerely,

Gregory Valentine
EES-5 Acting Group Leader

Cv: Peter Lichtner, MS C305