# United States Department of the Interior

U.S. GEOLOGICAL SURVEY
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MEMORANDUM

To: David Parkhurst, Lakewood, CO
From: Paul Barlow, Northborough, MA
Subject: Colleague review—"PHAST Version 2—A program for simulating groundwater flow, solute transport, and multicomponent geochemical reactions," by Parkhurst and others.

David,

Thank you for the opportunity to review the subject draft report. This is a comprehensive report that is, overall, well organized and well written. I've made several comments within the body of the report (electronically, using yellow highlighting and 'sticky notes') and have just a couple of major comments that are summarized below. You'll see that I did not do much editing of the report; in fact, the report doesn't need much editing in my opinion.

(1) Abstract, page 2: The PHAST code is a comprehensive flow, solute-transport, and reactive-transport simulator. The code is somewhat unique in my opinion because unlike many of the codes developed within WRD, grid- and input-data generation are more tightly integrated with the numerical-simulation process than is more normally the case, as evidenced, for example, by the options for defining grids, zones, and properties for a PHAST simulation. Also, the optional use of both grid- and map- coordinate systems, and the integration of Geographic Information System (specifically ArcInfo) data formats (shapefiles and text raster files) into the PHAST data-input structures, is fairly unique. Although you mention some of these issues in the Abstract, I think this aspect of the code should be discussed a little more in the Abstract and Introductory sections of the report.

Also, are shapefiles and text raster files (and other GIS data formats used in the report) unique to ArcInfo, or are they generic types of files that are used widely by GIS packages? I ask this because there seems to me to be an implicit endorsement of ArcInfo as a GIS package in the use of PHAST. If these are generic file types, then I think a statement should be added somewhere in the report that states that the files can be generated by any type of GIS package, and that ArcInfo is simply being referenced because of the familiarity of the authors with the ArcInfo system. This seems to me to be a USGS policy issue that I can't speak definitively about but recommend that you discuss the issue with a Publications Chief or Bureau Approving Official.

(2) First reference to Appendix D (Theory and Numerical Implementation): It's not clear to me why the theory and numerical implementation of the PHAST code are discussed in an Appendix. To me, these are fundamental components of the code that should be discussed prior to the input files and sample problems. Much of the information described in later sections of the report relates, not surprisingly, to the underlying theory of the code and requires an understanding of the theory (such as details on the grid and boundary conditions used in a PHAST simulation). In fact, I jumped ahead and read Appendix D immediately after reading the Introduction (Chapter 1) because I felt I needed to read the theory before the particulars of running the code. I understand this approach also was used in the version 1 documentation (TM 6-A8), but, again, it's not clear to me why this approach was used.

(3) Description of Keyword Data Blocks, beginning with section 4.5 Description of Input for Zones: I found the structure of these sections initially very confusing. After some reflection, I think what confused me was the intermingling of Examples and Explanations, and the placement of Examples before the Explanations within each data block. For example, the last part of the definition of '*zone*' within the **CHEMISTRY_IC** block (as well as in several other locations) is the sentence 'Line 1 defines a box zone.' I assume that what is meant is 'In the above example, line 1 defines a box zone.' Although I realize that this structure for the data-input descriptions also was used in version 1 of the report, I think it would make more sense to define the full scope of what is in each block before providing specific examples for each input block.

I was also initially confused by the use of Line numbers, which for most of our codes are used to describe specific input-item lines. I had to go back to the Documentation Conventions section to remind myself that the numbered lines in each example and subsequent explanation really have no meaning beyond a local connection between each example and subsequent explanation.

Also, the two examples in **HEAD_IC** lead me to wonder if all of the input options are fully described in the text for each input block. For example, example 1 in the **HEAD_IC** section has:

**HEAD_IC**
*zone*
**-head** *property*

and example 2 has:

**HEAD_IC**
**-water_table** *property*

do these identifiers and other input variables fully describe the possible contents of a **HEAD_IC** block? In my opinion, all possible input formats should be described for each input block in the report.

Finally, it seems to me that much of the text that is provided in the Notes for each keyword data block is basic background about the input block that could be placed in the introductory section for each data block. For example, I would consider all of the material in the Notes section for the **DRAIN** data block to be essential background material about how drains are simulated in the code and represented in the input blocks. Therefore, I would have expected this information to be provided before the line-by-line explanations of input requirements for the block.

(4) The Examples section is quite helpful and provides a lot of useful information. One of the benefits of the examples is that they illustrate the many ways that the input data can be defined in the data-input blocks. The discussions about numerical and natural dispersion are also very useful. Please see my comment on page 178 about the possibility of adding text describing the run times for each of the sample problems.

Please don't hesitate to contact me if you have any questions on these summary comments or those made in the body of the report.