This document briefly describes the content of the revised input specification, the rationale behind its development, and identifies issues that are still under discussion. Feedback is solicited on all aspects of the input spec, but in particular, those noted as not having been finalized.

General Description:

1. Our guiding principles for developing the new input spec were primarily
   1. The ability to validate the input data with the xml schema
   2. User-readability (eliminated the redundant Parameter List)
   3. Consistent use of attributes and elements in each section of the input file
2. In general, attributes were used to improve legibility and reduce verbosity. However, elements were used when it improved the ability to validate with the XML schema.
3. In general, major sections were defined in the plural, and individual elements in the singular (e.g., *<materials>* defines the major section, and *<material>* defines an element within it.)
4. Previously, values of the same type (e.g., BC times) were specified in horizontal lists, which was difficult to read when lists were long (e.g., aligning BC values with times). These quantities are now specified on the same line as their times to improve readability.
5. We combined the Time Period Control and Execution Control sections into a single Section labeled *execution\_controls*.  This improves readability, and eliminates the need to specify transient or steady-state with each control. .
6. XML does not require brackets around lists.  These were removed, and parentheses were used only for specifying coordinates.
7. The phase specification was maintained so that when Amanzi incorporates additional phases, those inputs can be easily incorporated into the spec.
8. Comments have been added to each major section. This was added because if a file is read in by Akuna, comments are not maintained when Akuna writes a new input file. In this way, the annotations to the input file will remain.

Major Section Descriptions

1. *model\_description*: This section is mostly unchanged, except for the addition of a default unit specification. If a non-default unit is specified in the file (currently only changes to time units are supported), then a space follows the unit. For example, <time> 1960 y</time>
2. *definitions*: This is a new section that defines all macros, and any named constants. These constants can be used for time or value specification. Note that the times in the macros are listed as elements, rather than as comma delimited lists. This is verbose, but since comma delimited lists cannot be validated against the XML schema, verbosity was preferred.
3. *process\_kernels*: The inputs specified here previously resided under the Execution Control section. Note that the transport algorithm is specified here, though technically it is a numerical control. Same is true of the chemistry.
4. phases: This section replaces the Phase Definitions from the previous spec. Same data is contained in this section as before. Element lists of solutes and solids appear here for XML validation (rather than a comma-delimited list).
5. *execution\_controls:* For clarity, numerical controls were separated into three different sections: 1) steady-state, 2) transient and liner solver. In this way, “steady-state” and “transient” aren’t needed for like parameters.
6. *mesh*: This block contains the same data as the previous input spec. The “unstructured” key word was eliminated because it appears at the top of the file under <amanzi\_input>.
7. regions: Two different ways of specifying regions are currently proposed. One is preferred for specifying regions defined by a filename, and the other is preferred for describing regions by shape (e.g., point, box, etc.). The latter has been distinguished using an element called <region\_list>. Supporting the two specifications is still under debate.
8. *geochemistry*: Geochemical <constraints> are listed under the geochemistry block. These specified conditions, once equilibrated, can be applied as initial and boundary conditions. Feedback is needed on the input structure for all aspects of geochemistry:
   1. In the example F-Area XML input file, minerals and their surface areas and volume fractions are specified under the constraints. These were placed here because they are considered to be part of the geochemical condition, as an aqueous concentration can be constrained by the presence of a mineral. Previously, the mineral volume fractions and surface areas were assigned in the <materials> section of the input file.
   2. In the example F-Area XML input file, the initial guesses for total concentration are specified. In the external Alquimia (pflotran) file (not provided), the secondary species, the ion activity model, the mineral kinetic rate parameters, site density for surface complexation, and the cation exchange capacity are specified. This arrangement splits the geochemical condition into two separate files, which may be confusing for the user. The data can all be consolidated into the external Alquimia file, and that filename only specified (included) in the Amanzi XML file. However, if any of this data is used by Agni, it should be explicitly written to the Amanzi input file. Which data is written to each of these files still needs to be finalized.
9. *materials*: This section contains the same data as before, except that mineral data has been moved to the geochemical section of the input file. Horizontal/vertical and anisotropy key word specification has been removed, and the user is required to specify permeability in the x, y and z directions.
10. *initial\_conditions*: Contains the same data as before. Named geochemical conditions are specified for both aqueous and solid phases, even though they may name the same condition.
11. *boundary\_conditions*: Contains the same data as before. Named geochemical conditions are specified for both aqueous and solid phases, even though they may name the same condition.
12. output: Contains the same data as before for observations and visualization.