Appendix C: Functionality Not Tested

For BRAGFLO Version 4.00, the following features will not be tested at this time because they will not be used as part of the WIPP compliance calculations:

1) Radionuclide transport. BRAGFLO is no longer used for transport calculations because a faster, more accurate, and more versatile code, NUTS, is now available.

2) Gas dissolution. Dissolution of gas in brine may be simulated using either Henry's law for a single gas or bubble point tracking. The brine may be specified as initially gas-free or fully gas-saturated. This feature will not be used in the WIPP compliance calculations and will not be tested now.

3) Numerous options are available for inputting the description of the mesh. Because only a couple of these are regularly used, the only ones that will be tested now will be those that will be used in the WIPP compliance calculations and in test cases for testing other features.

4) Reaction path gas generation model. This model has been neither fully developed nor implemented and is not available for the WIPP compliance calculations.

5) Multicomponent gas transport. Without a source of multiple gas components (i.e., the reaction path model), there is little point in tracking multiple gas components; this will not be done in the WIPP compliance calculations.

6) Three-dimensional calculations. Although BRAGFLO is a fully 3-D code, time and resource constraints currently preclude doing any 3-D calculations for WIPP compliance.

7) Three earlier creep closure surfaces. Creep closure data used for preliminary performance assessments have been retained in BRAGFLO to enable these calculations to be reproduced, but only the most recent creep closure surface (which became available in January 1996) will be used for WIPP compliance calculations.

8) Alternative equation solvers. In addition to the original LU solver, BRAGFLO also has a Linpack LU solver and a point-SOR iterative solver. The Linpack LU solver offers no advantages over the original LU solver, except for certain debugging capabilities. Because it has been coded very inefficiently, nearly doubling the memory required by BRAGFLO when it is used, it has been disabled in version 4.00. No iterative solver has yet been found that is sufficiently robust for calculations done for WIPP PA; in particular, the point-SOR solver is inadequate for use in the compliance calculations. An iterative multigrid solver is under development, but is not yet available for testing.

9) Capillary pressure treatment. An option in BRAGFLO is to allow the maximum capillary pressure to vary automatically. This model is experimental, has not been well-tested, and will not be used in the WIPP compliance calculations.

10) Numerical control parameters. The experience gained over several years of using BRAGFLO (see WIPP PA, 1991, 1992; NAS 1993 report; SPM1 1994; SPM2, 1995; FEPs Screening, 1995) has shown what values of the various control parameters will

enable BRAGFLO to run successfully. Test cases show that these values are being used as intended in the code. However, because the values of these parameters will not be varied in the WIPP compliance calculations, further testing is not done.

11) Multicomponent gas properties. BRAGFLO is capable of calculating gas properties using either the ideal gas law or the Redlich-Kwong-Soave equation of state. Properties can be calculated for either pure gases or for mixtures of any of the following six gases: H_2, CO_2, CH_4, N_2, O_2, and H_2S. Because the WIPP compliance calculations will use pure hydrogen and the Redlich-Kwong-Soave equation of state, the calculation of mixture properties and use of the ideal gas law are not tested.

12) Restart capability. This feature is used only for debugging and will not be used for the WIPP compliance calculations.

13) Relative permeability and capillary pressure models. BRAGFLO currently has 10 relative permeability and capillary pressure models available. Only two of these are expected to be used for the WIPP compliance calculations, KRP = 1 and 4; these will be tested for software QA. Three others (KRP = 5, 9, and 10) are used in QA testing, so these will also be tested. None of the other five models will be tested at this time.

14) Radiolysis (the radiolytic breakdown of water into hydrogen and oxygen) may be calculated. The initial inventory of radionuclides in the waste is input, and BRAGFLO calculates the decay of this inventory over time, along with the amount of water that is decomposed and the amount of gas generated. This feature will not be used in the WIPP compliance calculations and will not be tested now.

15) Certain little-used options for inputting the mesh are not tested. For parameter IDZFLAG, which specifies how Δz is input, options 2, 3, and 4 are not tested. (IDZFLAG options that are tested include 0 and 1.) For parameter IDEPTHFLAG, which specifies how the grid block elevations are input, options 1, 2, 3, 4, 5, 6, and -1 are not tested. (IDEPTHFLAG options that are tested include 0, -2, -3, and 7.) All available options for parameters IDXFLAG and IDYFLAG, which specify how Δx and Δy are input, are tested.