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Supplementary Material

INTEGRATION OF GEOCHEMISTRY INTO A GEOMECHANICAL SUBSURFACE FLOW SIMULATOR

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Appendix A: B5, Complex Geochemistry under Advection and Diffusion Transport

Benchmark 5 (B5), the most complex 1D model, includes advective and diffusive transport, dissolution, precipitation, and redox reactions, altering flow properties. It shares the same fluid and mineral contents as B3, but also includes diffusion as a transport mechanism.

B3 results are compared with reference models (MIN3P, TOUGHREACT, and porousMedia4FOAM). **Figure 1S** illustrates pressure and mineral volume fractions at 10, 100, and 300 years. The color code for simulators match those in B1, with solid lines for 10 years, dashed for 100 years, and solid with cross marks for 300 years. MF3D-GC results follow a similar trend to other simulators, while discrepancies increase gradually over the time because of accumulating differences in flow properties. Despite these minor differences, all simulated results show good agreement in pressure and mineral volume fractions.

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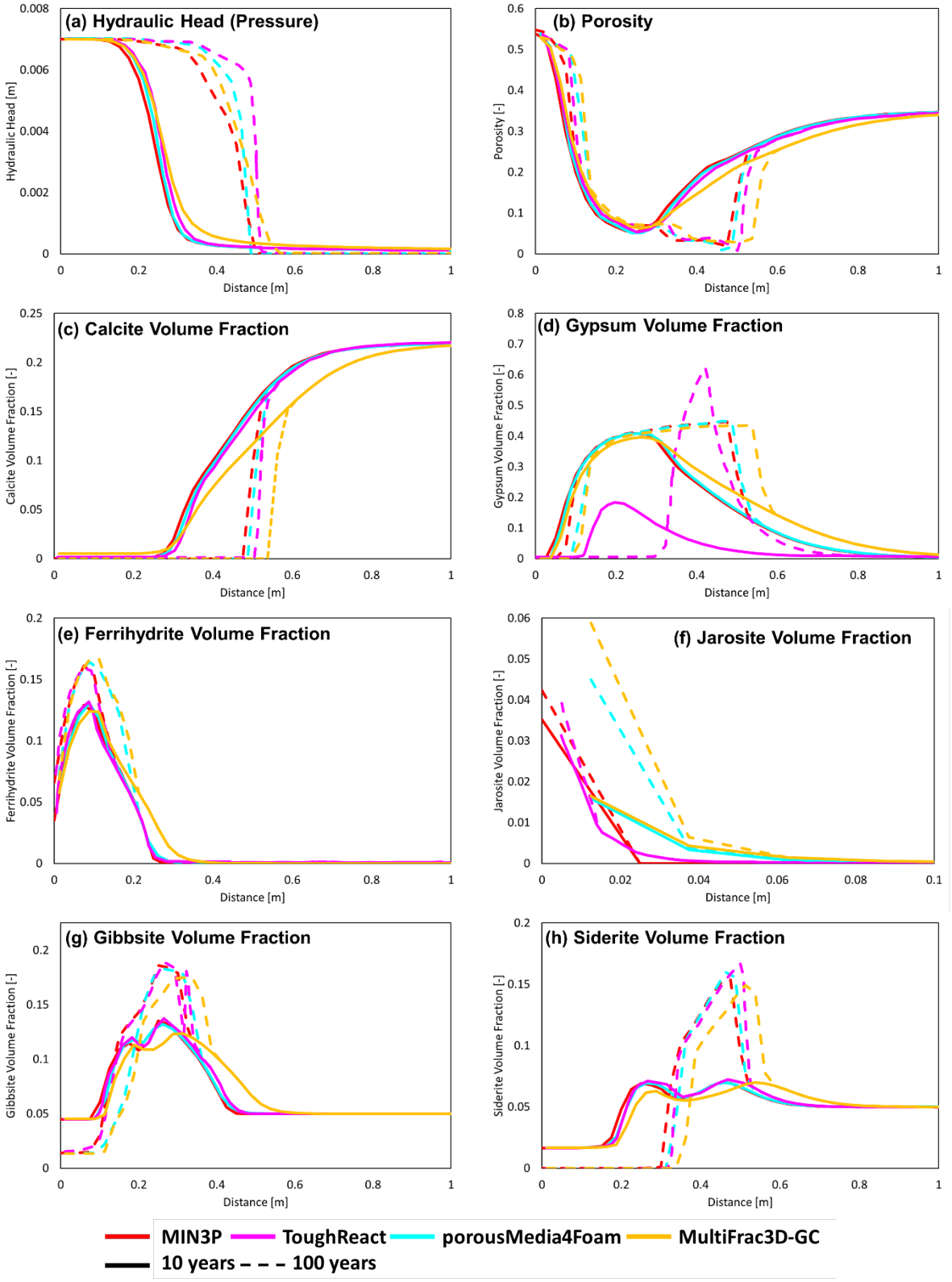

Figure 1S: Comparison of profiles (B5) of pressure **(a)** and porosity **(b)**, volume fraction of Calcite **(c)**, Ferrihydrite **(d)**, Gibbsite **(e)**, Gypsum **(f)**, and Jarosite **(g)** at 10, 100 and 300 years simulated by MIN3P, TOUGHREACT, porousMedia4Foam (PM4F), and MF3D-GC.

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