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Henry' law and gaz phase disappearance solved as a complementarity problem

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In a two-phase (liquid-gas) two-component (water-hydrogen) system we discuss the formulation of the possible dissolution of hydrogen in the liquid phase. The problem is formulated as a set of nonlinear partial differential equations with complementary constraints and we show how Henry's law fits in a phase diagram. Furthermore we show how this complementarity problem can be solved using nonsmooth Newton iterations. The problem is arising in a deep underground repository where hydrogen is produced by the corrosion of nuclear waste packages and we show our first numerical results.

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