Summary Statements

Physical and chemical dissolution-front instability problems exist ubiquitously in many scientific and engineering fields. In geoenvironmental engineering, the remediation of contaminated sites using fresh water to flush the contaminated soils involves propagation of the dissolved contaminant front in the water-saturated porous medium. In mineral mining engineering, the extraction of minerals in the deep Earth using the in-situ leaching technique may result in propagation of the dissolved mineral front in the fluid-saturated porous medium. In petroleum industry, the secondary recovery of oil by acidifying the oil field to uniformly increase porosity and hence the yield of oil is associated with propagation of the acid-dissolved material front in porous rocks. Thus, a systematical study on the dynamic mechanisms of physical and chemical dissolution-front instability phenomena is beneficial not only for understanding ore forming mechanisms, which are imperative to develop advanced techniques for exploring new ore deposits in the deep Earth, but also for understanding dissolved contaminant transport, which is important to develop innovative techniques for rehabilitating contaminated soils. Toward this end, both theoretical analyses and computational simulations have been extensively carried out in such a systematical study. As a result, the following conclusions have been drawn from the research work reported in the monograph.

(1) To solve chemical dissolution-front propagation problems, it is necessary to deal with a coupled system between porosity, pore-fluid pressure and reactive chemical-species transport in fluid-saturated porous media. Due to the morphological instability of a chemical dissolution front, this problem needs to be solved mathematically and numerically. Mathematical methods are used to establish a theoretical criterion for assessing whether or not a chemical dissolution system under consideration is in a critical or supercritical state. A segregated algorithm based on a combination of the finite element and finite difference methods has been proposed for

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simulating the morphological evolution of chemical dissolution fronts in chemical dissolution systems of critical and supercritical Zhao numbers. A set of analytical solutions have been derived for a benchmark problem to verify the proposed numerical procedure. Not only can the derived analytical solutions be used to verify any numerical method before it is used to solve this kind of chemical dissolution-front propagation problem, but also they can be used to understand the fundamental mechanisms behind the morphological instability of a chemical dissolution front during its propagation within fluid-saturated porous media of critical and supercritical Zhao numbers. The related numerical results have demonstrated that the proposed segregated algorithm and related numerical procedure are useful for and capable of simulating the morphological instability of chemical dissolution fronts within fluid-saturated porous media.

(2) The related theoretical and numerical results from investigating the effects of particle reactive surface areas have demonstrated that: first, since the shape coefficient of spherical grains is greater than that of cubic grains, the chemical dissolution system consisting of spherical grains is more unstable than that consisting of cubic grains; second, the instability likelihood of a natural porous medium, which is comprised of irregular grains, is smaller than that of an idealized porous medium, which is comprised of regular spherical grains; third, reactive surface areas associated with different particle shapes can have a significant influence on the morphological evolution of an unstable chemical-dissolution front within the fluid-saturated porous medium.

(3) The related theoretical results from investigating the effects of mineral dissolution ratios have revealed that the mineral dissolution ratio plays an important role in controlling the propagation speed of a planar chemical dissolution-front in the fluid-saturated porous medium. An increase in the value of the mineral dissolution ratio can result in a remarkable decrease in the value of the dimensionless propagation speed of a planar chemical dissolution-front. On the other hand, the related computational simulation results have demonstrated that the mineral dissolution ratio has a considerable influence on the evolution pattern of a planar chemical dissolution-front during its propagation in the fluid-saturated porous medium. An increase in the mineral dissolution ratio can reduce the likelihood for a planar chemical dissolution-front to evolve from the initial planar shape into different morphologies within the fluid-saturated porous medium of finite size.

(4) The theoretical results from examining the effects of solute dispersion have led to the following findings. First, the propagation speed of a planar chemical dissolution-front in the case of considering solute dispersion effects is exactly the same as that when solute dispersion effects are neglected. This indicates that solute dispersion does not affect the propagation speed of the planar chemical dissolution-front in a fluid-saturated porous medium. Second, consideration of solute dispersion can cause a significant increase in the critical Zhao number, which is used to

judge whether or not a planar chemical dissolution-front may become unstable in the fluid-saturated porous medium. This means that the consideration of solute dispersion can stabilize a planar chemical dissolution-front because an increase in the critical Zhao number reduces the likelihood of the planar chemical dissolution-front instability in a fluid-saturated porous medium. Third, for both a given solute dispersion ratio and a given longitudinal dispersivity, an increase in the final porosity value destabilizes the chemical dissolution-front so that it becomes easier for a planar chemical dissolution-front to evolve into different morphologies. In addition, the present results can be used as benchmark solutions for verifying numerical methods employed to simulate detailed morphological evolution processes of chemical dissolution fronts in two-dimensional fluid-saturated porous media.

(5) The related theoretical and numerical results from investigating the effects of medium permeability anisotropy have clearly demonstrated that a decrease in the medium anisotropic permeability factor (or ratio), which is defined as the ratio of the principal permeability in the transversal direction to that in the longitudinal direction parallel to the pore-fluid inflow direction, can stabilize the chemical dissolution front so that it becomes more difficult for a planar chemical dissolution-front to evolve into different morphologies in the chemical dissolution system. On the other hand, the medium anisotropic permeability ratio can have significant effects on the morphological evolution of the chemical dissolution front. When the Zhao number of the chemical dissolution system is greater than its critical value, the greater the medium anisotropic permeability ratio, the faster the irregular chemical dissolution-front grows.

(6) The related theoretical and numerical results from examining the effects of pore-fluid and medium compressibility have led to the following findings. First, not only can pore-fluid compressibility affect the propagation speeds of chemical dissolution fronts in both subcritical and supercritical chemical dissolution systems, but also it can affect the growth and amplitudes of irregular chemical dissolution fronts in supercritical chemical dissolution systems. Second, medium compressibility may have a little influence on the propagation speeds of chemical dissolution fronts, but it can have significant effects on the growth and amplitudes of irregular chemical dissolution-fronts in supercritical chemical dissolution systems. Third, both medium and pore-fluid compressibility may stabilize irregular chemical dissolution-fronts in supercritical chemical dissolution systems.

(7) To simulate the chemical dissolution-front evolution in a three-dimensional fluid-saturated porous medium, a combined numerical procedure consisting of the finite difference and finite element methods has been proposed. Since the problem belongs to a complex system science problem, a small randomly-generated perturbation of porosity is added into the initial porosity of a three-dimensional homogeneous domain to trigger the instability of a planar chemical dissolution-front during its propagation

within the fluid-saturated porous medium. To test the correctness and accuracy of the proposed numerical procedure, a three-dimensional benchmark problem has been constructed and the related analytical solution has been derived. This enables the proposed numerical procedure to be used for simulating the morphological evolution of a three-dimensional chemical dissolution-front from a stable, planar state into an unstable, fingering state. The related numerical results have demonstrated that the proposed numerical procedure is useful for and capable of simulating the morphological evolution of a three-dimensional chemical dissolution-front within the fluid-saturated porous medium.

(8) A theoretical criterion for assessing the instability of planar NAPL dissolution-fronts in two-dimensional fluid-saturated porous media of finite domains has been established. Not only can the present theoretical results be used for theoretical understanding of the effect of solute dispersion on the instability of a NAPL dissolution front in the fluid-saturated porous medium of either a finite domain or an infinite domain, but also they can be used as benchmark solutions for verifying numerical methods employed to simulate the detailed morphological evolution processes of NAPL dissolution fronts in two-dimensional fluid-saturated porous media. The related simulation results have revealed that: (i) the proposed numerical procedure is useful and applicable for simulating the morphological evolution of NAPL dissolution fronts in two-dimensional fluid-saturated porous media of finite domains; (ii) if the Zhao number of a NAPL dissolution system is in the lower range of the supercritical Zhao numbers, the fundamental mode is predominant; (iii) if the Zhao number is in the middle range of the supercritical Zhao numbers, the (normal) fingering mode is the predominant pattern of the NAPL dissolution front; and (iv) if the Zhao number is in the higher range of the supercritical Zhao numbers, the fractal mode is predominant for the NAPL dissolution front.

(9) The related numerical simulation results from investigating the effects of domain shapes have demonstrated that: (i) domain shapes have a significant effect on both the propagation speed and the morphological evolution pattern of a NAPL dissolution front in the fluid-saturated porous medium; (ii) an increase in the divergent angle of a trapezoidal domain can lead to a decrease in the propagation speed of the NAPL dissolution front; (iii) the morphological evolution pattern of the NAPL dissolution front in a rectangular domain is remarkably different from that in a trapezoidal domain of a large divergent angle; (iv) for a rectangular domain, the simplified dispersion model, which is commonly used in the theoretical analysis and numerical simulation, is valid for solving NAPL dissolution instability problems in fluid-saturated porous media; and (v) compared with diverging flow (when the trapezoidal domain is inclined outward), converging flow (when the trapezoidal domain is inclined inward) can enhance the growth of NAPL fingers, indicating that pump-and-treat systems by extracting contaminated groundwater might enhance NAPL

dissolution fingering and lead to less uniform dissolution fronts.

(10) The propagation theory of mesh discretization errors associated with a NAPL dissolution system is first presented for a rectangular domain and then extended to a trapezoidal domain. This leads to the establishment of the finger-amplitude growing theory associated with both the corner effect and the mesh discretization effect in the NAPL dissolution systems of trapezoidal domains. This theory can be used to make the approximate error estimation of the corresponding computational simulation results. The related theoretical analysis and numerical results have demonstrated that: (i) both the corner effect and the mesh discretization effect can be quantitatively viewed as a kind of small perturbation so that they can have some considerable effects on the computational results of supercritical NAPL dissolution systems; (ii) the proposed finger-amplitude growing theory associated with the corner effect at the entrance of a trapezoidal domain is useful for correctly explaining why the finger at either the top or the bottom boundary grows much faster than that within the interior of the trapezoidal domain; and (iii) the proposed finger-amplitude growing theory associated with the mesh discretization error in the NAPL dissolution system of a trapezoidal domain can be used for quantitatively assessing the correctness of computational simulations of NAPL dissolution-front instability problems in trapezoidal domains, so that it can be ensured that the computational simulation results are controlled by the physics of the NAPL dissolution system, rather than by the numerical artifacts.

(11) The intrinsic time is used to determine the time scale at which the acidization dissolution front is formed, while the intrinsic length is used to determine the length scale at which the instability of the acidization dissolution front can be initiated. Under the assumption that the acidization dissolution reaction is a fast process, the critical Zhao number, which is used to assess the instability likelihood of an acidization dissolution-front propagation in fluid-saturated carbonate rocks, has been derived in a strictly mathematical manner. Based on the proposed instability theory of a propagating acidization dissolution front, it has been theoretically recognized that: (i) the increase of the mineral dissolution ratio can stabilize the acidization dissolution front in fluid-saturated carbonate rocks; (ii) the increase of the final porosity of the carbonate rock can destabilize the acidization dissolution front, while the increase of the initial porosity can stabilize the acidization dissolution front in fluid-saturated carbonate rocks; (iii) the increase of the mineral dissolution ratio can cause an increase in the dimensionless propagation speed of the acidization dissolution front; and (iv) the increase of the initial porosity can enable the acidization dissolution front to propagate faster, while the increase of the final porosity can enable the acidization dissolution front to propagate slower in the acidization dissolution system.

(12) At the end of this monograph, it needs to be pointed out that there remains much to be done in this particular research field. For instance, only physical and chemical dissolution fronts of planar shapes are treated theoretically in this field. Physical and chemical dissolution fronts of other different shapes, such as circular, cylindrical and spherical shapes, have not been theoretically considered so far. In addition, temperature effects in non-isothermal dissolution systems have also neglected in the current research. To solve energy shortage problems facing the mankind, physical and chemical dissolution-front instability phenomena should be employed to develop advanced and innovative techniques for extracting unconventional hydrocarbons, such as gas hydrates, heavy oil, and shale oil/gas, from the reservoirs that are comprised of low porosity rocks.

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