

Changling inorganic carbon dioxide gas field in Songliao Basin, China

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Changling gas field is located in Chaganhua town in Qianguo county, Jilin province. Geotectonically, it is located in the uplift of volcanic belt in the central region of Changling fault depression, southwest Songliao Basin. Gas pays lie in the Lower Cretaceous Yingcheng Formation volcanic rocks. It is an important carbon dioxide gas field with 4 drilled wells, being of controlled reserves of tens of billions cubic metres and controlled gas bearing areas of 8.39 km².

The main geochemistry characteristics of deep gases in the fault depression are listed as follows: (1) The gases are characterized by high CO₂ except Changshen 1 well (CO₂ accounts for 20.05%). Of the main components of gases in Changshen 1 well, CH₄ accounts for 71.99%, the hydrocarbon gases above C₂ account for 1.37%, He and N₂ account for 0.023% and 6.35%, respectively. In the Changshen 1-1 and Changshen 1-2 wells, the contents of CH₄ are within the range of 22.26% ~ 29.71%, and the contents of hydrocarbon gases above C₂ are within the range of 0.20% ~ 0.26%. The contents of H₂, He, CO₂ and N₂ are within the ranges of 0.05% ~ 0.84%, 0.0076% ~ 0.012%, 71.64% ~ 67.46% and 4.24% ~ 1.53%, respectively. It was proposed that a gas field with CO₂ more than 60% could be called carbon dioxide gas field (Dai *et al.*, 2005), therefore the Changling gas field is a carbon dioxide gas field. (2) The ranges for the $\delta^{13}\text{C}_1$, $\delta^{13}\text{C}_2$, $\delta^{13}\text{C}_3$ and $\delta^{13}\text{C}_4$ values of the gases from Changling gas field are -22.2‰ to -23.4‰, -26.3‰ to -27.0‰, -26.5‰ to -27.3‰ and -33.3‰ to -34.0‰, respectively. It is a significant character for inorganic hydrocarbon gas that the $\delta^{13}\text{C}$ values are getting lighter with increasing molecular weight (Dai *et al.*, 2005), so the hydrocarbon gases in this field are inorganic. The $\delta^{13}\text{C}_{\text{CO}_2}$ values of CO₂ from Changling gas field are within the range of -6.8‰ to -11.9‰. It has been pointed out that CO₂ with $\delta^{13}\text{C}_{\text{CO}_2} > -8\text{‰}$ is inorganic (Dai *et al.*, 2005). Most of the CO₂ from this field has $\delta^{13}\text{C}_{\text{CO}_2}$ greater than -8‰, so it is inorganic. (3) In Changling gas field, the ranges of ³He/⁴He and R/Ra values are 2.61×10⁻⁶ to 3.21×10⁻⁶ and 1.90 to 2.10, respectively. The ³He/⁴He values in the upper mantle and radioactive strata are within the range of 1.1×10⁻⁵~1.4×10⁻⁵ and 10⁻⁷~10⁻⁹, respectively (Wang, 1989). The ³He/⁴He values of He from this field are around 10⁻⁶, which indicates a large amount of ³He from the mantle. All these evidences demonstrate that the gases from Changling gas field are mainly inorganic.

References

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Kink sites: A key to surface reactivity and dissolution kinetics

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Dissolution and corrosion of crystalline materials have been proven to be as complex as they are important. In recent years significant progress in our understanding of dissolution mechanisms and kinetics was based on experimental studies utilizing atomic force microscopy (AFM), interferometry (e.g., VSI and PSI) and other techniques. Building on the rapidly growing power of computers, these efforts have been complemented by computer models of rapidly increasing sophistication and complexity. *Ab initio*, DFT, Molecular Dynamics (MD), and lastly Monte Carlo (MC) calculations are contributing to an increasingly detailed picture of reaction kinetics in complex systems [1].

Here, we apply parameterized Monte Carlo simulations to explore dissolution kinetics at critical time and length scales, over which experimental and analytical tools have limited utility or feasibility as sources of precise information [2]. The system size that can be explored with MC simulations is now sufficiently large to permit realistic predictions of surface alteration and dissolution mechanisms that can then be verified experimentally. We use results from *ab initio* and DFT calculations to parameterize our calculations.

Lasaga [2] demonstrated that the arrival and departure rates (*k*) of atoms or molecules are equal at surface kink sites only when the crystal surface is at equilibrium, thus:

$$k_{+}^{\text{kink}} = k_{-}^{\text{kink}}$$

The kink site is indeed the most important reactive site at a crystal surface, because a molecule in this position has precisely half the chemical bonds that it would have were it located in a bulk site. At the same time, a kink site is the only *self-replicating* site at a given crystal surface.

Our MC calculations use the ability to study kink site dynamics from a molecular (versus purely geometric) basis, and are case studies for crystal systems. When combined with a statistical treatment, our MC results demonstrate that the large amount of detailed information involved in the complex problem of surface reactivity, and its role in overall kinetics of dissolution can be significantly reduced by focusing primarily on the number, type, and density of kink sites and their development over time and space.

References

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