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煤储层不同尺寸孔中H_2O对CH_4解吸扩散的分子模拟研究

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The Molecular Simulation of the Influence of H_2O on CH_4 Desorption and Diffusion in Pores with Different Size of Coal Reservoirs

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摘要/Abstract

摘要：

模拟煤储层中甲烷(CH_4)在不同孔径中不同水分下的解吸和扩散过程，讨论孔径、含水率、温度和压力与CH_4解吸扩散的关系。结果表明，狭缝的壁面叠加效应会显著影响H_2O分子的吸附/解吸，使H_2O分子集中分布在狭缝孔的中间位置。当孔间距逐渐增大时，双侧壁面叠加效应逐渐转化为单侧壁面的表面效应对H_2 O分子的吸附，使H_2O分子的分布由中间转为两边。含水率的增加对CH_4解吸的影响程度增加，CH_4的解吸量呈减小趋势，但受温度影响规律不明显。在1nm狭缝孔中，低压时的水分对CH_4解吸的影响程度大于高压下的情况。在2nm狭缝孔中，当含水率由2.35%增加至5%时，低压时的水分对CH_4解吸的影响程度则开始小于高压下的情况。在5nm狭缝孔中，随着压力的降低，含水率对CH_4解吸量的影响变得不明显，说明在解吸过程中，压力降到某一值后，改变含水率并不会促进CH_4的解吸；当含水率超过2.35%时，含水率的增加仍然对CH_4的解吸产生影响，说明2.35%并不是石墨狭缝孔的水分临界值，但由于随着含水率的增加，CH_4所受的影响程度逐渐变小，因此临界值可能存在。微孔中水的吸附热和微孔对吸附质分子的强吸附势使孔径和含水率显著影响CH⌟4的扩散系数，而温度和压力对CH_4的扩散系数则影响较小。

关键词: 煤层气, 含水率, 孔径, 解吸, 扩散, 分子模拟

Abstract:

Desorption and diffusion of methane (CH_4)under different moistures in different size pores of coal reservoirs were simulated.The relationships between pore size,moisture,temperature,pressure and desorption/diffusion of CH_4 were discussed.The results show that (1)the wall superimposed effect of the pore can significantly affect the adsorption/desorption of H_2O molecules,so H_2O molecules concentrate distribution in the middle of the pore.With increase of pore size,the wall superimposed effect of the pore gradually transforms into surface effect of two sides of the wall so that H_2O molecules concentrate distribution on both sides|(2)With the increase of the moisture content,the influence of the moisture on CH_4 desorption capacity increases,and CH_4 desorption capacity shows a trend of decrease,but the temperature effect is not obvious|(3)In the 1nm slit pore,the influence of the moisture on CH_4 desorption under low pressure is greater than that under high pressure|(4)In the 2nm slit pore,when the moisture content increases form 2.35% to 5%,the moisture impact on CH_4 desorption under low pressure is less than that of high pressure|(5)In the 5nm slit pore,with the decrease of pressure,the influence of the moisture content on CH_4 desorption capacity becomes not obvious,which explains that when the pressure drops to a certain value,changes of the moisture content will not promote CH_4 desorption.When the moisture content is more than 2.35%,the increase of the moisture content still affect CH_4 desorption,which explains that 2.35% is not the moisture critical value of the graphite slit pore.However,with the increase of the moisture content,CH_4 desorption is less affected gradually,so the critical value may exist|(6)Adsorption heat of water in micropores and adsorption potential from micropores to adsorbates will significantly affect the diffusion coefficient of CH_4,while temperature and pressure less affect it.

Key words: Coalbed methane, Moisture content, Pore size, Desorption, Diffusion, Molecular simulation

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