Natural gas (NG) coming from reservoir often contains a significant fraction of undesirable compounds such as water. Under certain temperature and pressure conditions, the presence of water in gas pipelines can lead to formation of natural gas hydrates that pose a risk of pipeline blockage. To prevent hydrate formation, water is removed from the natural gas. Triethylene glycol (TEG) is commonly used in the petroleum industry for natural gas dehydration to meet transport and sales gas specifications. Adsorption of water on molecular sieves (zeolites) is a technique commonly used for deep water dew point depression. Regeneration of the adsorbent can be performed by either heating, pressure reduction or a combination of the two. While necessary to free up the adsorption sites, the process of regeneration will also result in deterioration of the adsorbent, which has to be replaced after a number of adsorption-regeneration cycles. A too-frequent replacement of adsorbent incurs heavy costs; any insights into ameliorating the situation would be beneficial. When considering the factors that may contribute to a premature deterioration of industrial adsorbents, one must also consider that a certain amount of TEG may follow the water into the zeolite during adsorption and affect the zeolite framework either directly or indirectly. To investigate the impact that TEG adsorption into LTA zeolites will have on zeolite interactions with water at different temperatures, a range of Molecular Dynamics (MD) simulations have been performed. Evaluation of TEG models with respect to the enthalpy of vaporization, diffusivity and other physical properties have been performed. More complex MD simulation studies of composite systems containing LTA Zeolite, water and TEG, as well as methane have been conducted at different temperatures and initial conditions.