The incorporation of phase change materials (PCMs) into building elements is an effective technique that has been gaining momentum in the construction industry for achieving reductions in the energy consumption of buildings. The operation of PCM-incorporated building elements has been widely proven experimentally; however fundamental problems are encountered when it comes to its numerical simulation, where non-linear phenomena that change in time and space also have to be considered. This paper reviews the existing literature on the numerical simulation of PCMs for building applications, and identifies the basic parameters that are required to be taken into account for conducting the numerical simulation of PCM-incorporated building systems. These parameters include the geometry and discretization of the simulated PCM-incorporated building system, the physics of heat transfer embracing thermophysical properties and heat transfer mechanisms, and boundary conditions to be considered for the numerical simulation, and the implementation of experimental validation studies. The focus of this paper is to provide evidence for the significance of considering heat convection to the calculation of the thermal performance of PCM. In view of the findings of the literature review, numerical studies for a building wall incorporating PCM are conducted. The results of the simulation studies assess the impact and emphasize the importance of accounting for natural convection within the liquid PCM in numerical simulation studies.