

Comparison of pseudo-component and multi-component approaches in mixture release

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There have been many leakage accidents of chemicals. For example, mixture of hydrogen chloride and toluene was leaked from valve at Yeosu in 2005, and hydrochloric acid was released from tank at Sangju in 2013. In the case of pure components, release simulation is easier and more accurate than mixture because the property data is already equipped, however, mixture calculation is rather complex. There are two methods of calculating mixture's thermodynamic behaviors and properties: pseudo-component (PC) approach and multi-component (MC) one. The former method computes properties by averaging the pure substances with respect to composition. While, the latter one works out more rigorous result using flash calculation. In chemical release simulators, such as Phast or CARIS, most of mixture properties are calculated by PC approach. In this study, the results of PC and MC approaches are compared and suitability of PC approach in simulators is analyzed.