Proceedings of the 5th World Congress on Momentum, Heat and Mass Transfer (MHMT'20)
~~Lisbon, Portugal~~ Virtual Conference – October, 2020
Paper No. ICMFHT 183
DOI: 10.11159/icmfht20.183

Numerical Study of Single Iron(III) Nitrate Nonahydrate/Ethanol Droplet Evaporation in Humid Air

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Abstract **-** The heating and evaporation of spherically symmetric droplets consisting of a precursor solution of iron(III) nitrate nonahydrate (INN) and ethanol for nanoparticle synthesis in spray flames is studied numerically. The multicomponent droplets are at standard conditions and the evaporation is initiated through the elevated temperature of the convective ambient air. The liquid mixture properties of INN and ethanol used in the model are fits to new experimental data which are valid in the temperature range of 293.15 K through 333.15 K and for mass fractions of INN in ethanol up to 0.34. In general, there are two different pathways through which the nanoparticle synthesis may occur from the precursor solution. In the first pathway, the particle forms directly inside the liquid precursor solution, and in the second pathway, the droplet is transferred entirely into the gas phase from which the nanoparticle may form. The INN/ethanol precursor droplet is treated as a three-component solution consisting of ethanol, iron(III) nitrate, and water, where the INN consists of the latter two. The process is initially governed by the ethanol evaporation and later by water evaporation since ethanol is more volatile component. Further decomposition and liquid-phase reactions may occur inside the precursor droplet, eventually leaving over an iron (III) nitrate particle or transferring the iron (III) nitrate into the gas phase, which happens beyond the thermal decomposition temperature of 403 K beyond which the iron (III) nitrate may decompose into gaseous Fe_2O_3, so that the entire INN/ethanol droplet transforms into the gas phase. The study presents simulations of the evaporation of the INN/ethanol droplet for both situations.

Keywords**:** multicomponent droplet evaporation, thermal decomposition, precursor solution, iron(III) nitrate nonahydrate, ethanol, numerical study