Numerical Study of Thermal Evaporation Unit for Phase Change of Liquid Hydrogen Peroxide to Vapor

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Abstract

model was required.

Hydrogen peroxide (H2O2) vapor is a preferred medium of sterilization in different fields of industry. Among the fact that it dissociates to oxygen and water (environmentally-friendly) [1], H2O2 vapor possesses strong mircobicidal and sporicidal characteristics [2, 3]. As such, the use of H2O2 vapor as a sterilant has continuously increased in different fields of industry, like in medicine, pharma and food packaging. The described sterilization process requires a fully evaporated composition-homogenous stream of gaseous sterilant with a pre-defined flow temperature. Hence, an FEM tool was used to investigate a conceptual design of an evaporation unit (see Figure 1) for the phase change to gaseous form of an aerosol containing H2O2. Process parameters such as heating power defined as an input current to the meander-type heating element were examined. In addition, the design of the unit was investigated, in which a complete evaporation of a 35%-weight H2O2 solution is required at the outlet with a temperature of approximately 150 °C. Using COMSOL Multiphysics® software, a numerical model of the evaporator unit was realized, in which an aerosol mixture of 2 m³/h air and 3.6 L/h 35%-wt. H2O2 solution was applied as inlet parameter. The aerosol, assumed to be a homogeneous mole-averaged mixture, flows in a serpentine channel with 10 mm in diameter and 1.73 m in length. The channels holding the fluid are embedded in a steel structure of 20 cm in length and width and 25 mm in height. The physics describing the simplified evaporation model were summed up to be coupled effects of non-isothermal phase-changing fluid flow of turbulent nature, heat transfer in solids and electric current (shell approximation). Due to the conceptual design, no symmetry can be assumed for the geometry and therefore, a full 3D

To achieve a process-related depiction of the numerical model for the evaporation unit, the temperature and composition-dependent material properties were derived and applied. The enthalpy of vaporization and the region of temperature change for a binary H2O2-water mixture were calculated using vapor pressure equations derived by Schumb, Scatchard and Keyes [4, 5]. In this study, the steady-state response of the system was investigated. Therefore, a stationary solver with a combination of auxiliary sweep for current value was computed. The auxiliary sweep serves in smoothing the transition of physical properties over the defined transition phase to stabilize the solver. Figure 2 shows the temperature profile through the mid-section of the serpentine channel. A

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relatively constant temperature is observed at the highlighted section of the serpentine channel. This refers to the enthalpy required to change the phase and is an indication of the phase change phenomena. In Figure 3 the development of the gas phase is presented through various sections of the serpentine structure.

This study provides the initial step towards modeling of an H2O2 aerosol evaporator for chemical sterilization purposes. Geometric enhancement and further model extensions can be achieved to realize an efficient evaporation process and to apply best practical process parameters.

Reference

[1] P. A. Giguère and I. Liu, Kinetics of the Thermal Decomposition of Hydrogen Peroxide Vapor, Canadian Journal of Chemistry, Vol. 35(4), p. 283-293 (1957)
[2] M. Khadre and A. Yousef, Sporicidal Action of Ozone and Hydrogen Peroxide: A Comparative Study, International Journal of Food Microbiology, Vol. 71(2), p. 131-138 (2001)
[3] G. McDonnell, The Use of Hydrogen Peroxide for Disinfection and Sterilization Applications, Patai's Chemistry of Functional Groups, John Wiley & Sons, p. 1-34 (2014)
[4] G. Scatchard et al., Vapor-Liquid Equilibrium. VIII. Hydrogen Peroxide—Water Mixtures, Journal of the American Chemical Society, Vol. 74(15), p. 3715-3720 (1952)
[5] W. C. Schumb et al., Hydrogen Peroxide: Part Two, Cambridge, Mass: M.I.T. Depts. of Chemistry and Chemical Engineering (1953)

Figures used in the abstract

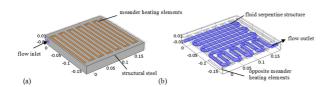


Figure 1: Model of the simulated evaporator unit showing (a) the solid domains of the model and (b) the fluid domain.

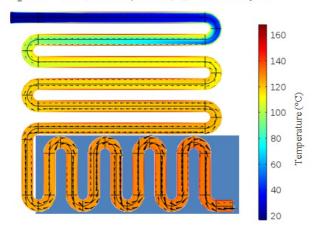


Figure 2: Temperature distribution in the serpentine for heating current of 185 A through the meander heating elements. Cone arrows indicates the direction of the flow (size proportional to flow velocity). Highlighted section shows a relatively constant temperature, which indicates most phase transition region.

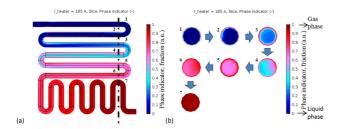


Figure 3: Cross-sectional view of (a) the aerosol's change of phase from liquid to vapor due to a heating current of 185 A indicating a phase change process that develops around the wall region, and (b) the homogeneity of the gaseous phase at different locations of the serpentine channel.