

# Numerical Simulation Of Cold Atmospheric Pressure Plasma Jet To Predict NO<sub>x</sub> Species Distribution

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## Abstract

Cold atmospheric pressure plasma (CAPP) is a novel technology that can be used as a surface treatment for food to make it microbiologically safe. CAPP is an ionized gas which consists of charged and neutral particles. Various reactive species such as reactive oxygen species and reactive nitrogen species in plasma can be effectively used for microbial inactivation. The amount and the type of reactive species mainly responsible for microbial inactivation vary with plasma generation method, feed gas, input energy, gas flow rate, humidity, and frequency of power supply. Prediction of microbial inactivation kinetics due to plasma and reproducibility of microbial inactivation is challenging because of complex chemistry of plasma. The possibility of numerically predicting the amount of reactive species distribution may help to predict microbial inactivation based on the reactive species.

The specific objectives of the research include development of a numerical model for (1) Fluid flow and heat transfer in the plasma jet, and (2) the transport of reactive nitrogen species (NO<sub>x</sub>) distribution in the jet and the substrate surface. Nitrogen species are main antimicrobial agents in the plasma jet responsible for microbial inactivation. In the long term, we will be able to correlate the reactive nitrogen species distribution with the microbial inactivation.

COMSOL Multiphysics® Heat transfer, CFD, and Chemical Engineering modules were used to perform numerical simulation of turbulent flow of air plasma along with heat transfer and charged species transport. The generation of reactive species and their decay were included in the simulation. The heat transfer and CFD (rotating machinery- turbulent flow) module were coupled in a three-dimensional domain to include cylindrical rotating jet (radius 0.4 cm and length 5 cm) and its surrounding domain (H=20 cm, W=20 cm, L=20 cm). The COMSOL Chemical Engineering module was used for transport of reactive species in the jet and on the substrate. For a stationary axisymmetric jet, the velocity at the nozzle exit was 4.8 m/s and the temperature was 407 K. Average predicted steady state NO<sub>x</sub> concentration at the substrate surface was about  $5 \times 10^{-12}$  mol/m<sup>3</sup>. Numerical simulation for a rotating jet is being conducted to predict flow profiles, temperature distributions, and NO<sub>x</sub> species distribution. The future work will include correlating the concentration of NO<sub>x</sub> with the microbial inactivation to predict microbial inactivation efficacy of the jet plasma process.