Mathematical modeling tools for practical chlorine control in produce wash process

SUMMARY

The produce wash stage has received much attention as a critical control point, however, recent studies indicate a limited understanding of the dynamics of sanitizer control during washing. One problem is that the relationships between water quality constituents and sanitizer levels have only been described via experimental/ correlative approaches or by risk models that are difficult to parameterize accurately. Accordingly, there is an urgent need to mathematically describe the fundamental dynamics that generate the observed relationships between sanitizer levels and water quality parameters. Based on such formulations, the primary objective of this proposal is to develop data-informed modeling tools which quantitatively link easily measurable water quality parameters to commodity specific organic load and free chlorine (FC) consumption during recirculated wash conditions. Based on USDA experimental data and our recent modeling results, we hypothesize that our modeling tools will provide the industry with predictive capabilities that are not possible using correlations alone.

OBJECTIVES

Main objective: To construct data-informed models which quantitatively link easy to measure water quality parameters to commodity specific organic load and FC decay kinetics during recirculated wash conditions.

The above objective will be realized via the following two tasks for carrots and green cabbage (various cut types for each produce kind), respectively.

Task 1: Build mathematical models describing wash water chemistry relative to commodity specific aspects.

Task 2: Validate model predictions against lab and pilot-plant scale data.

METHODS

The CSU team is currently conducting experiments and building predictive models focused on the lab scale:

Experiments
- Benchtop experiments are underway for various cut types of carrots/cabbage during simulated wash water process, with pH maintained at 6.5.
- Physiochemical quantities measured include FC, turbidity, TDS, pH, water temperature, and COD.
- Initial FC about 20 mg/L; maximum produce to water ratio is ~0.2 kg/L.

Modeling
- Statistical analysis, ordinary differential equations and parameter optimization techniques are being implemented to build "carrot/cabbage specific" models that allow prediction of COD levels via turbidity/TDS measurements at the lab scale relative to the amount of produce/liter washed.
- At the same time, the CSU team is utilizing chemical reaction and ordinary differential equation theory to construct FC decay modeling specific to carrots/ cabbage.
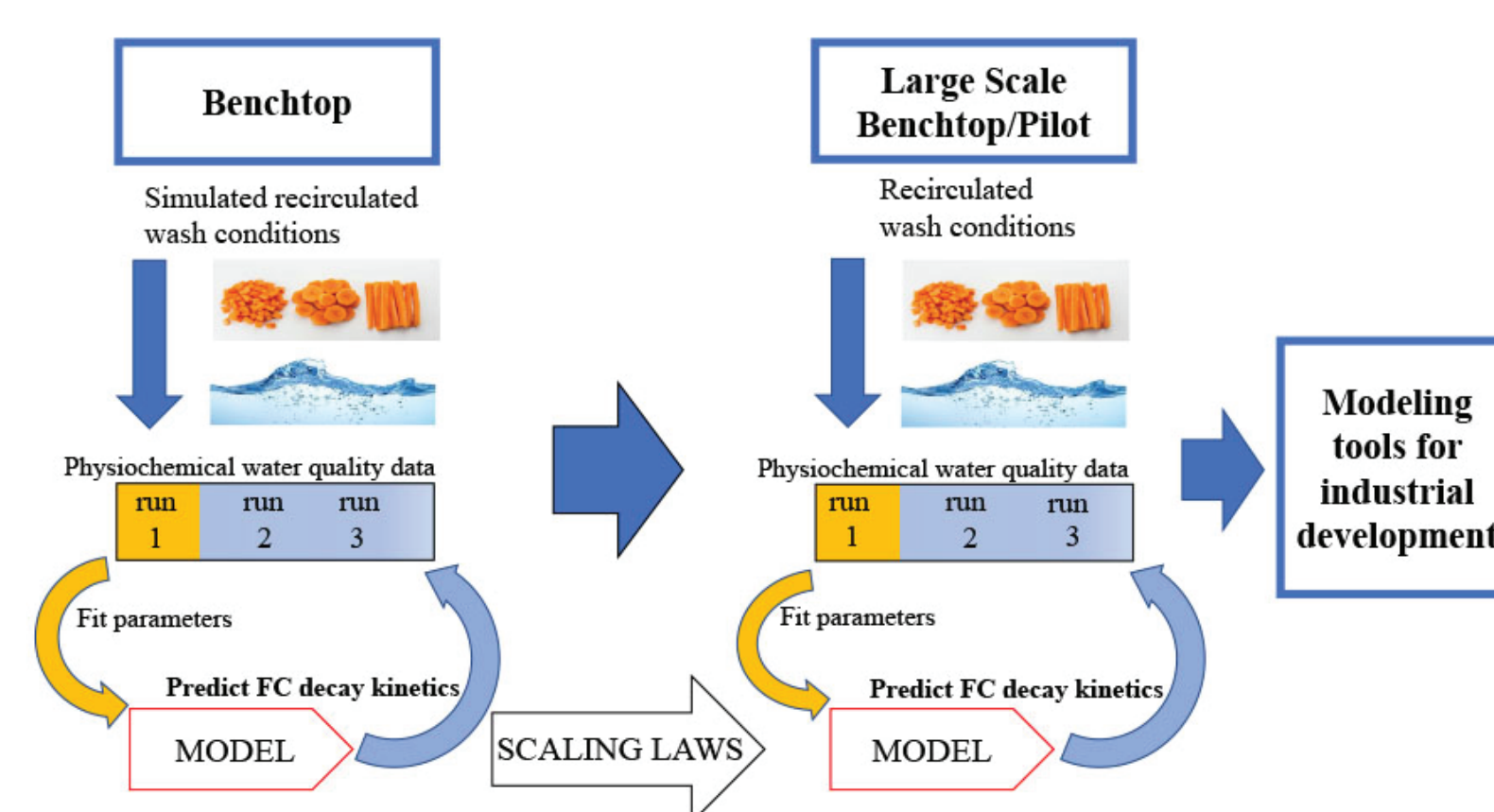
RESULTS TO DATE

- Sub-model which predicts COD via turbidity measurements at benchtop scale during stick cut carrot washing (Figure 3 & 4a)
- Mechanistic model predicting FC decay via turbidity measurements at benchtop scale during stick cut carrot washing (Figure 3 & 4b)
- Once benchtop experiments and modeling are completed, the project focus will move to large scale benchtop/pilot scale. This will be accomplished via experimental results from Yaguang Luo (USDA-ARS) and experiments at CSU (Figure 1 and 2).
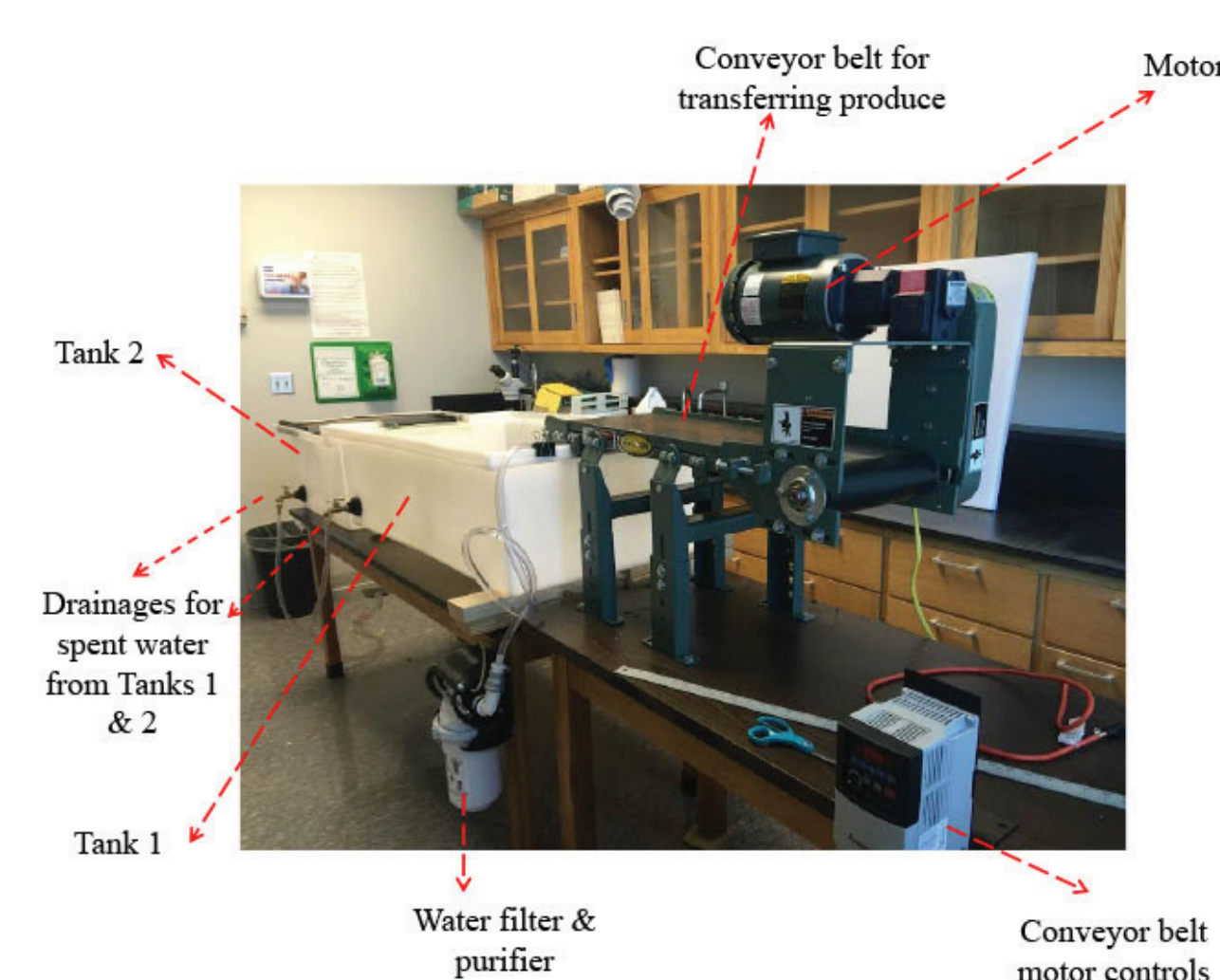
BENEFITS TO THE INDUSTRY

- Modeling tools can be used to help minimize FC variability during fresh-cut carrot/ cabbage washing.
- Results will illustrate the wash system risk associated to periodic/manual sanitizing schemes with sustained duration between doses.
- Model results will provide guidelines for further experimentation, streamlining the scope and frequency of expensive pilot-plant/commercial scale data acquisition.
- Model results will provide a basis for development of real-time control for sanitizer systems.

Figure 1. Logic flow for the project.

Figure 2. Setup for large-scale benchtop experiments; available tank capacity is 200– 500 L.

Figure 3. Equations describing a mathematical model to predict FC decay kinetics at the benchtop scale that is informed by real-time turbidity measurements. Y_n, and the specific form of f, can be adjusted to represent other water quality parameters such as TDS, UV254, etc.
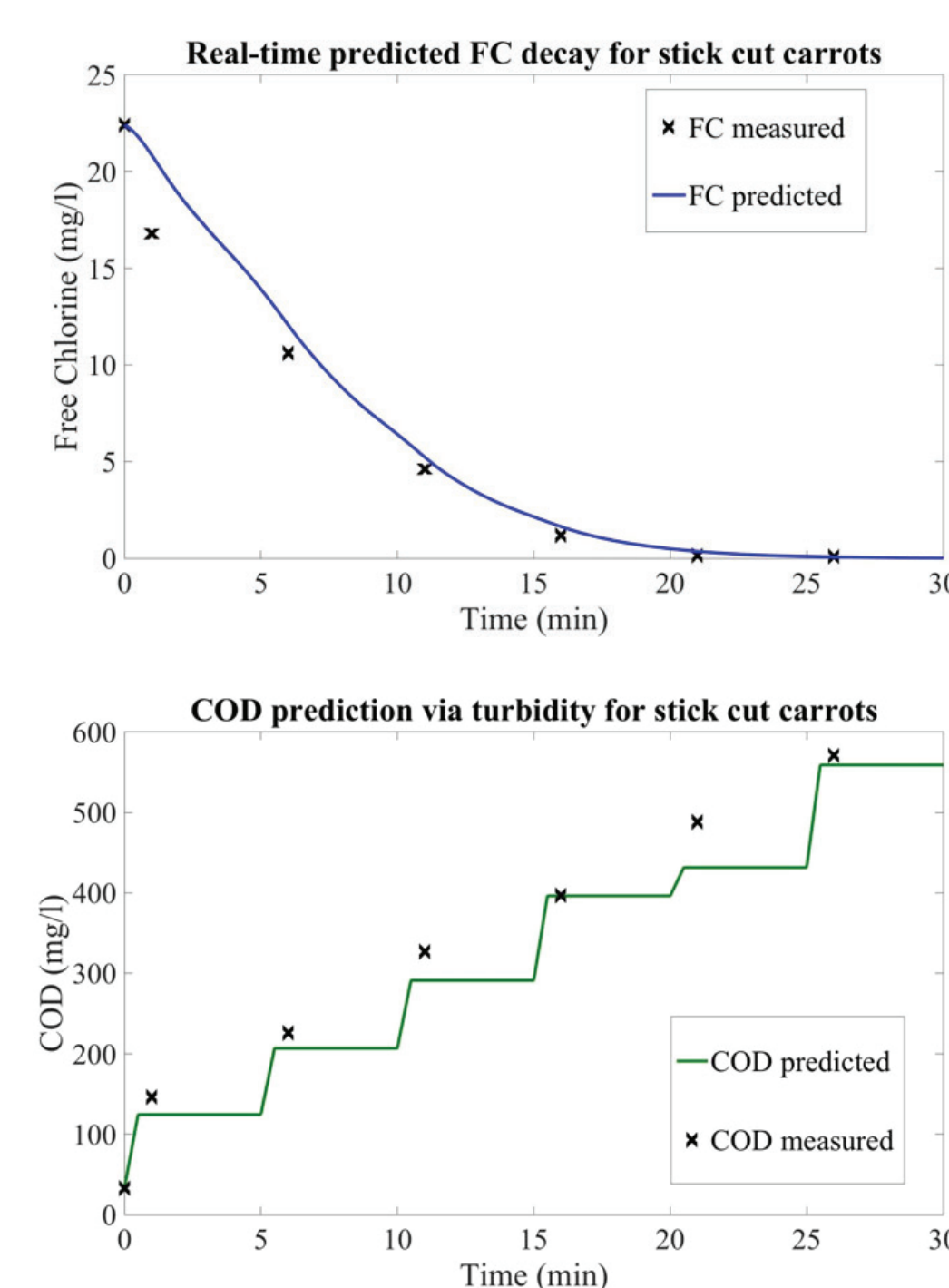
Mathematical model for free chlorine decay kinetics

$$\frac{dO}{dt} = \sum_{n=1}^{N} f\left(Y_n, \frac{dY_n}{dt}\right) \chi_{[t_{n-1}, t_n]}$$

$$\frac{dC}{dt} = -k_0 g(C) - k_1 h(O, C)$$

- O is the organic load in the wash tank quantified as COD (mg/l),
- C is the free chlorine concentration in the wash tank (mg/l),
- Y_n is the turbidity (or surrogate parameter) at time t_n, dY_n/dt is the change in turbidity, N total number of measurements,
- $f(Y_n, dY_n/dt)$ captures the real-time turbidity to COD prediction,
- χ is the indicator function, g and h are forms for chlorine reactions,
- k_0 is a chlorine reaction rate constant (function of temperature),
- k_1 is a chlorine reaction rate constant (function of pH and temperature).

Figure 4. a) COD prediction via the dO/dt equation in Figure 3. Note, dO/dt is updated only from turbidity measurements; R^2 =0.96. b) FC prediction via the dC/dt equation in Figure 3. The result depends on the dominant reaction rate constant k_1 = 0.00075 (l/(mg min)), determined from a different experimental run, and the corresponding turbidity measurements updating the dO/dt equation; R^2 = 0.96.

CONTACT

Daniel Munther
Department of Mathematics
Cleveland State University
T: 216-523-7184
E: d.munther@csuohio.edu

AUTHORS

a. Ryan Abnavi
b. Ali Alraadan
c. Anthony Sulak
d. Chandra Kothapalli (Co-PI)
e. Partha Srinivasan (Co-PI)
f. Daniel Munther (PI)

CPS CENTER for PRODUCE SAFETY