About me

Work experience

Assoc R&D Principal Scientist, PepsiCo

Postdoctoral Researcher, Turbomachinery Lab

Education

PhD, Mechanical Engineering, Texas A&M University

MS & BS, Mechanical Engineering, National Taiwan University

Hobbies

Travel

LEGO

Chao-Cheng (Joe) Shiau

How Modeling and Simulation Can Help Process Authority in Decision-Making?

Chao-Cheng (Joe) Shiau

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PepsiCo R&D

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Why and how does modeling and simulation come into the pictures?

Motivation: Process complexity

Methodology: M&S (CFD)

Use cases: Bottle rinsing, holding tube

Takeaway messages

Few questions about the process

- **Bottle rinsing**
  - How can we effectively rinse different bottle designs?
  - What are the important factors for the bottle rinsing?
  - Can we visualize the coldspot during rinsing?
  - Any measure for cleanliness comparison?
- **Holding tube**
  - How the holding tube design really affect the process?
    - Slopped upward/downward
    - Elbow
  - How does the slopped affect the holding time (residence time)
  - If there’s air entrapment happening in the holding tube, where is it?

Process complexity facilitates the idea for a more efficient way for process tunning and optimization

Parameters can be evaluated

Geometry: nozzle type (spray pattern), bottle design, holding tube length

Process: presence of sanitizer, flow rate, rinse/drain time, nozzle position, process/residence time

Efficacy

How do we know the process time is sufficient?
How do we know if the package is clean?
How do we know if the process is efficient?

Can computer models help the process authority in decision-making

Utilize modeling and simulation to make the process more efficient and effective

Costly and time consuming to physically test all parameters

→

Modeling and simulation (virtual testing) allows minimizing or replacing physical testings

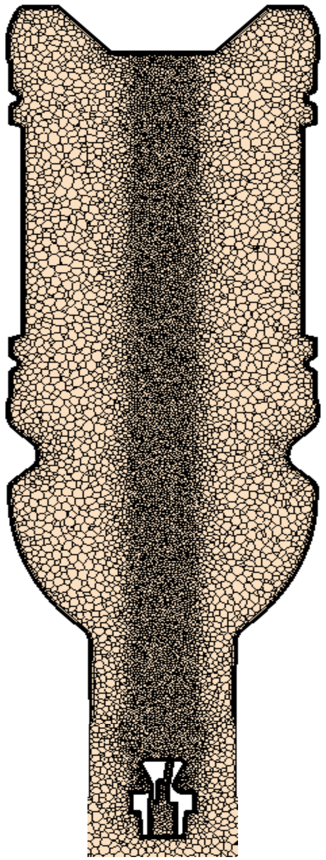
→

Better and faster decision-making

Bottle Rinsing Modeling

Methodology for the modeling and simulation (CFD)

Common procedure for modeling and simulation using the Computational Fluid Dynamics (CFD) technique



$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0$$

$$\rho \frac{\partial v}{\partial t} + \rho (v \cdot \nabla) v = \nabla \cdot [-p + (\mu + \mu_T) v] + \mu \nabla^2 v + f$$

$$\rho \frac{\partial k}{\partial t} + \rho (v \cdot \nabla) k = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right] + P_k - \rho \varepsilon$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho (v \cdot \nabla) \varepsilon = \nabla \cdot \left[\left(\mu + \frac{\mu_T}{\sigma_\varepsilon} \right) \nabla \varepsilon \right] + C_{1\varepsilon} \frac{\varepsilon}{k} P_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k}$$

- Domain discretization and fluid mechanics recreate physical processes in the virtual space

Use case 1: Package wet treatment/rinsing modeling

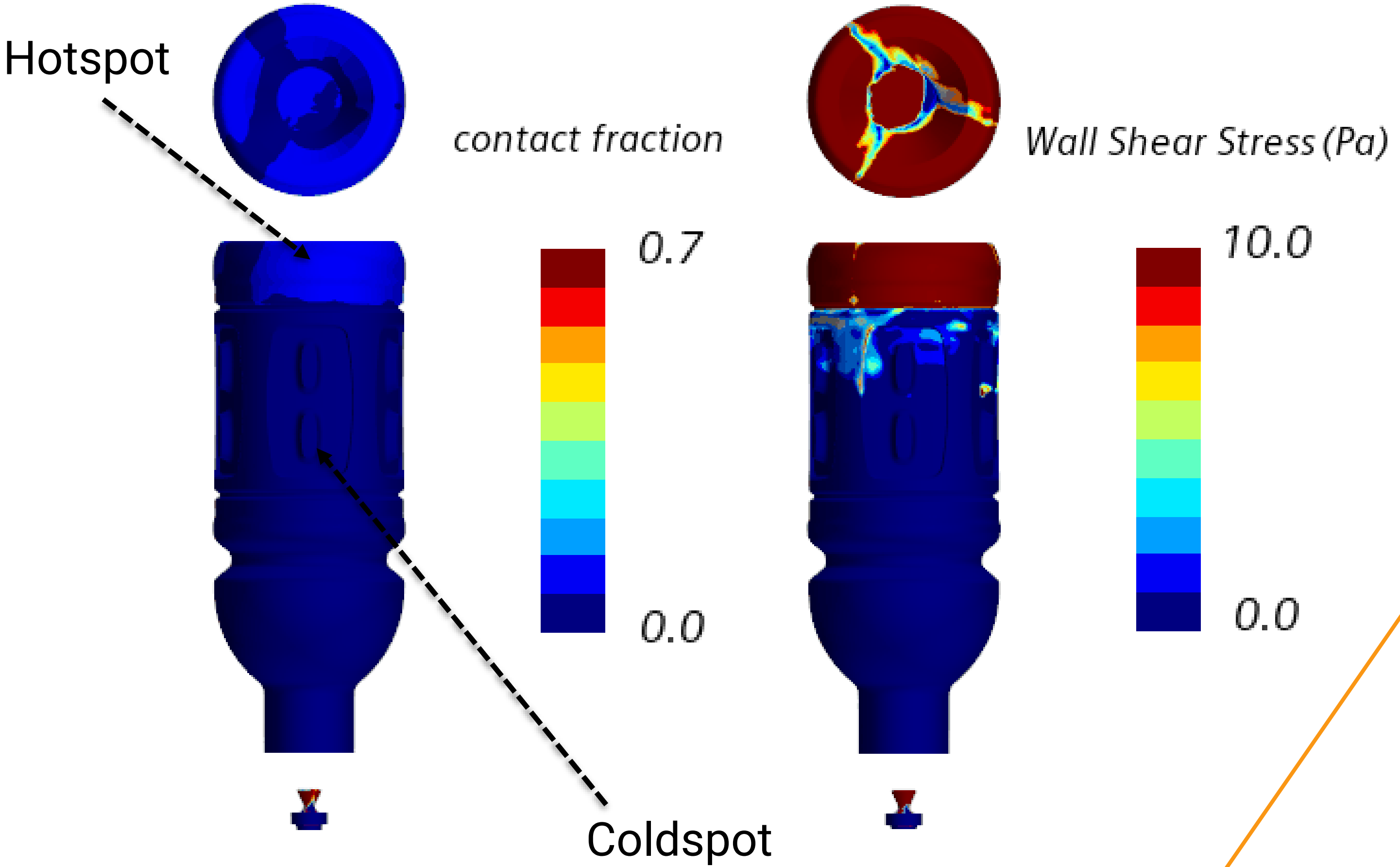
Problem statement:

Using CFD model to recreate the package rinsing process for **what if analysis** on coldspot comparison from varying rinsing pattern (nozzle), bottle design (shape), bottle and nozzle alignment.

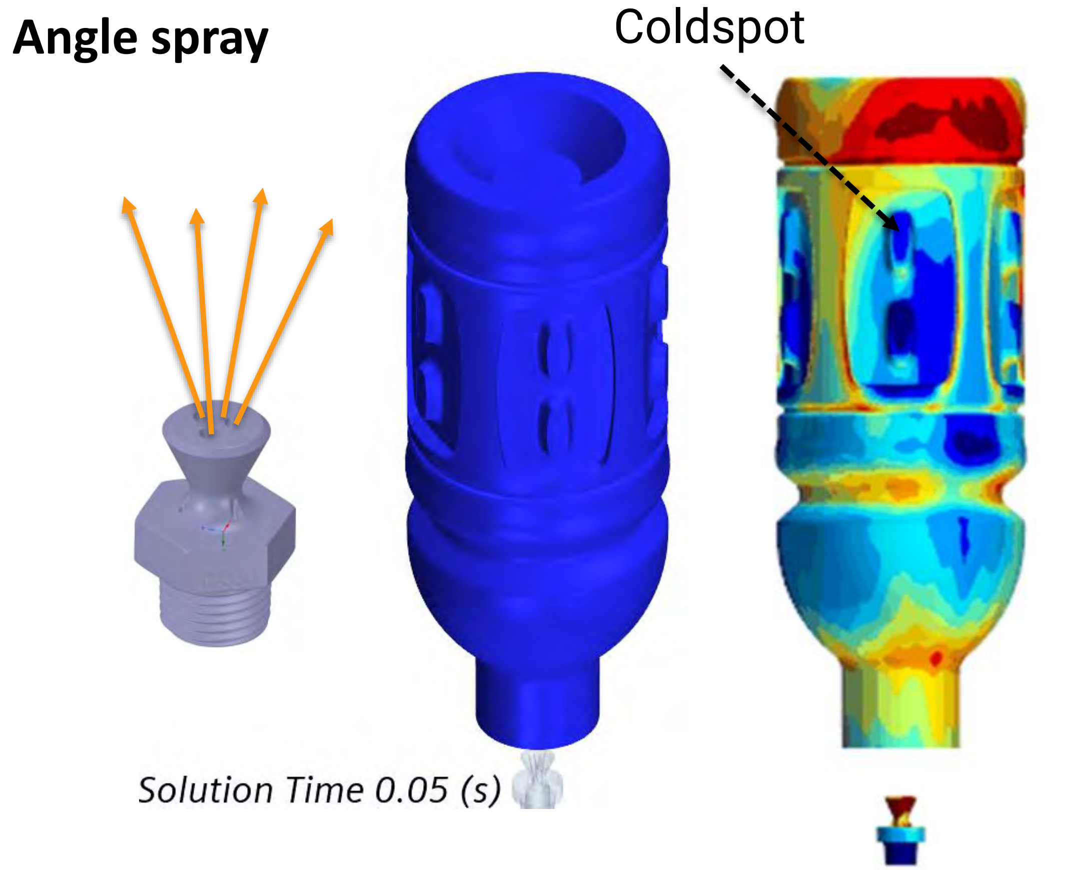
Package: 20 oz Bottle 1

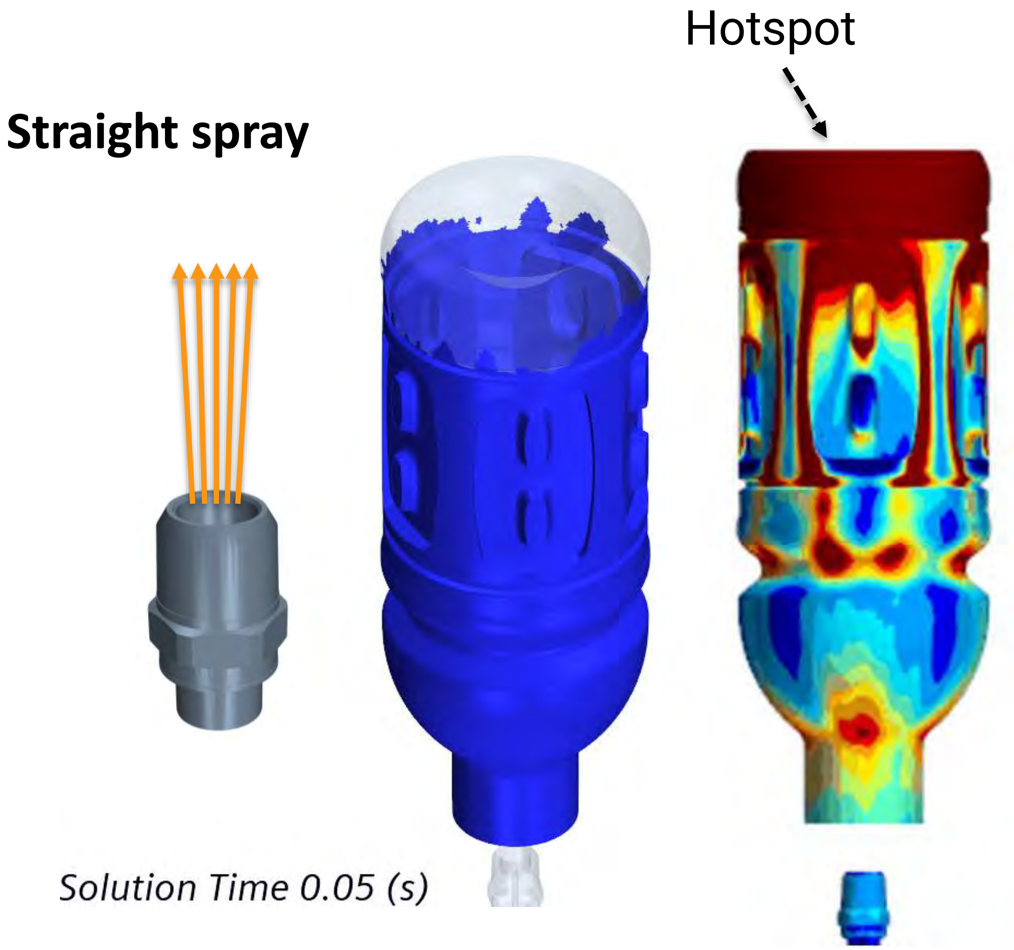
Nozzle type: Angle spray

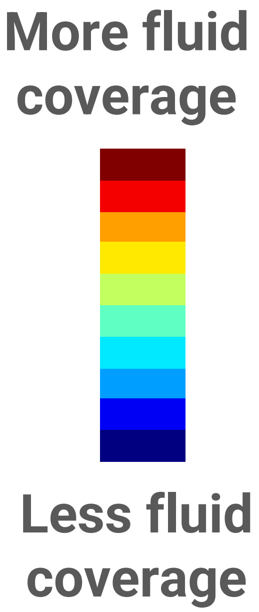
Flow rate: 1.8 gpm



What happen when you use different nozzle?



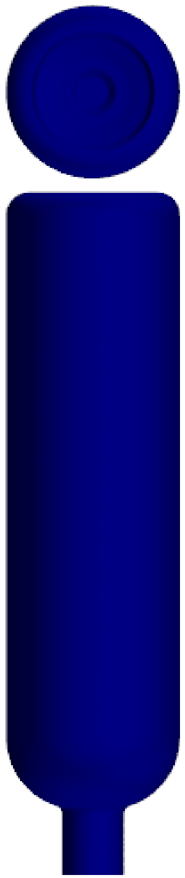




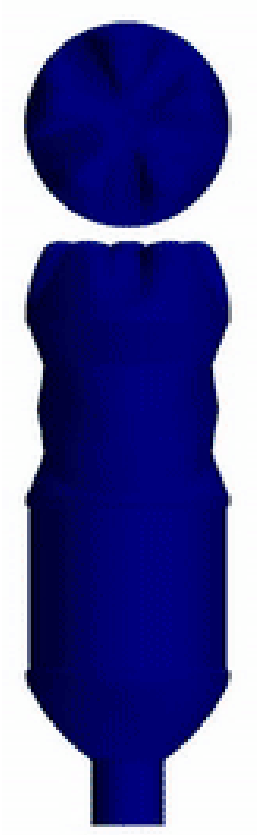
Straight spray leads to more liquid coverage and less cold area for this bottle design

What happen when we rinsing different bottle?

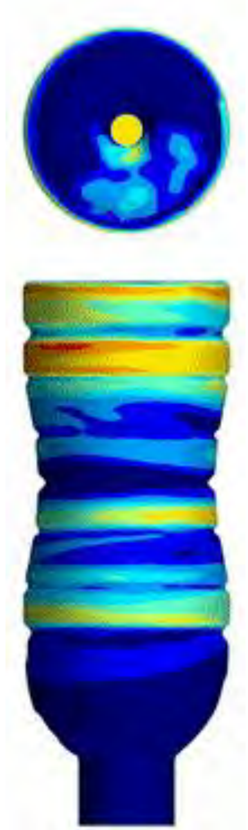
Bottle 1



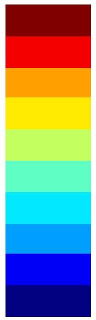
Bottle 2



Bottle 3



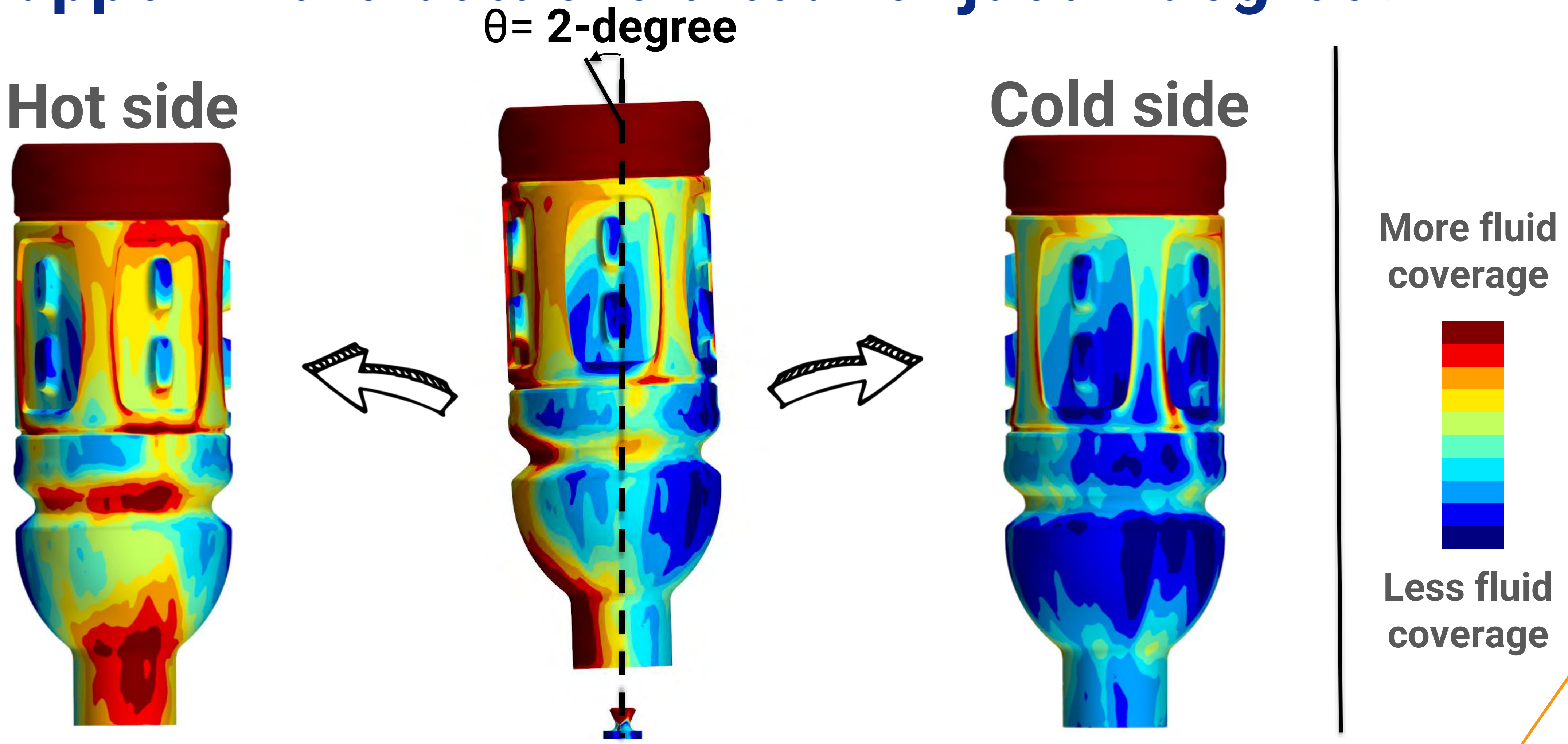
More fluid coverage



Less fluid coverage

For a given (the same) rinsing setting, different bottle design leads to different liquid distribution and cold area

What happen if the bottle is tilted for just 2 degree?



Bottle misalignment from vertical by 2-degree can lead to dramatically different liquid distribution

Takeaway from this case

- A rinsing model is developed

- This model allows quickly changing bottle and design, as well as the process condition to provide straightforward coldspot mapping as the directional guidance to process authority

Holding Tube Modeling

Use case 2: Holding tube modeling

Problem Statement

Using CFD model to study if a “sloped upward” holding tube (HT) does have **advantage** over flat HT in terms of

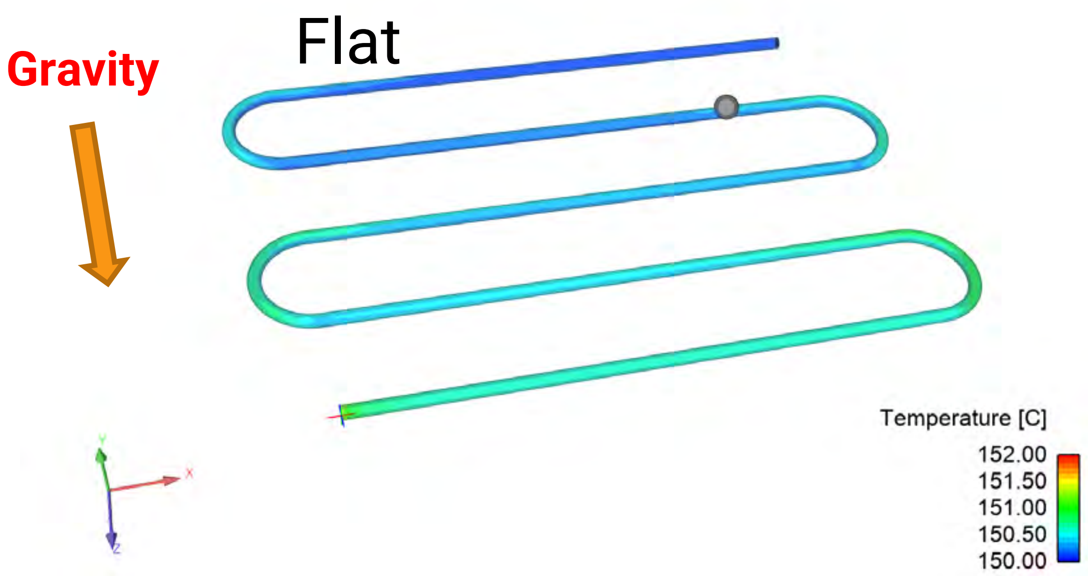
- **Uniform product flow**
- **Less air entrapment**

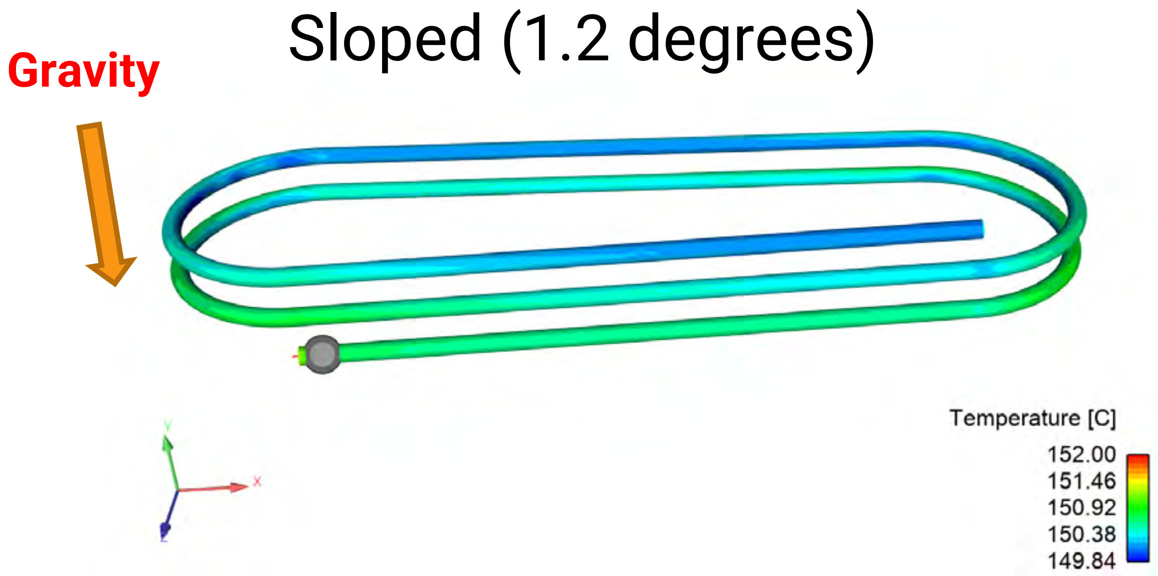
From FDA

21 CFR 113.40(G) The holding tube shall be designed so that no portion of the tube between the product inlet and the product outlet can be heated, and it must be sloped upward at least 1/4-inch per foot (2.1 centimeters per meter).

1.2 degrees

Comparison under the same tube length (13m), flowrate and properties (Re_D ~ 8,100, turbulent flow)





Method

In addition to the typical modeling methodology on p.8,

Assumptions:

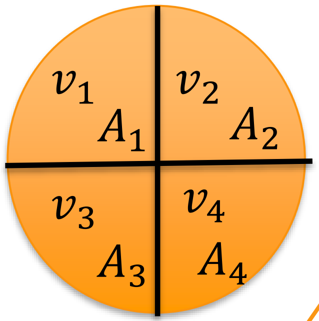
- Do you consider particulate in the flow?
  No
- Can velocity uniformity represent the uniform product flow?
  Reasonable if no particle in the flow (or particle does not change the bulk flow behavior due to it's size)

Let's assume uniform product flow in the HT correlates with the velocity uniformity

Use HT **outlet** as the monitoring plane, define the uniformity (γ_m) as

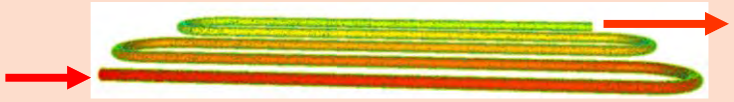
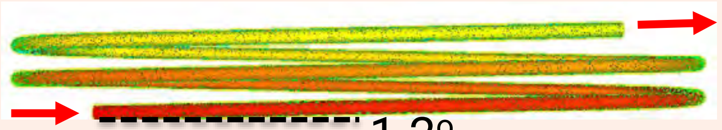
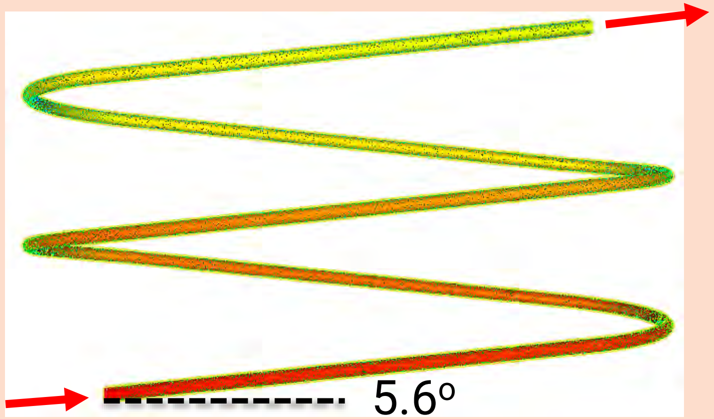
$$\gamma_m = 1 - \frac{\sum_{i=1}^{n}[(|v_i - \bar{v}_m|)(|\rho_i v_i A_i|)]}{2|\bar{v}_m|\sum_{i=1}^{n}[|\rho_i v_i A_i|]}$$

$$\bar{v}_m = \frac{\sum_{i=1}^{n}[v_i(|\rho_i v_i A_i|)]}{\sum_{i=1}^{n}[|\rho_i v_i A_i|]}$$



γ_m **= 1 -> uniform**
γ_m **= 0 -> nonuniform**

3 scenario HT study (at given flow condition)

Scenarios		Residence time	Uniformity (γ_m) at outlet
Flat HT		9.75	0.917
Sloped (1.2^o) HT		10.4	0.919
Sloped (5.6^o) HT		10.3	0.917

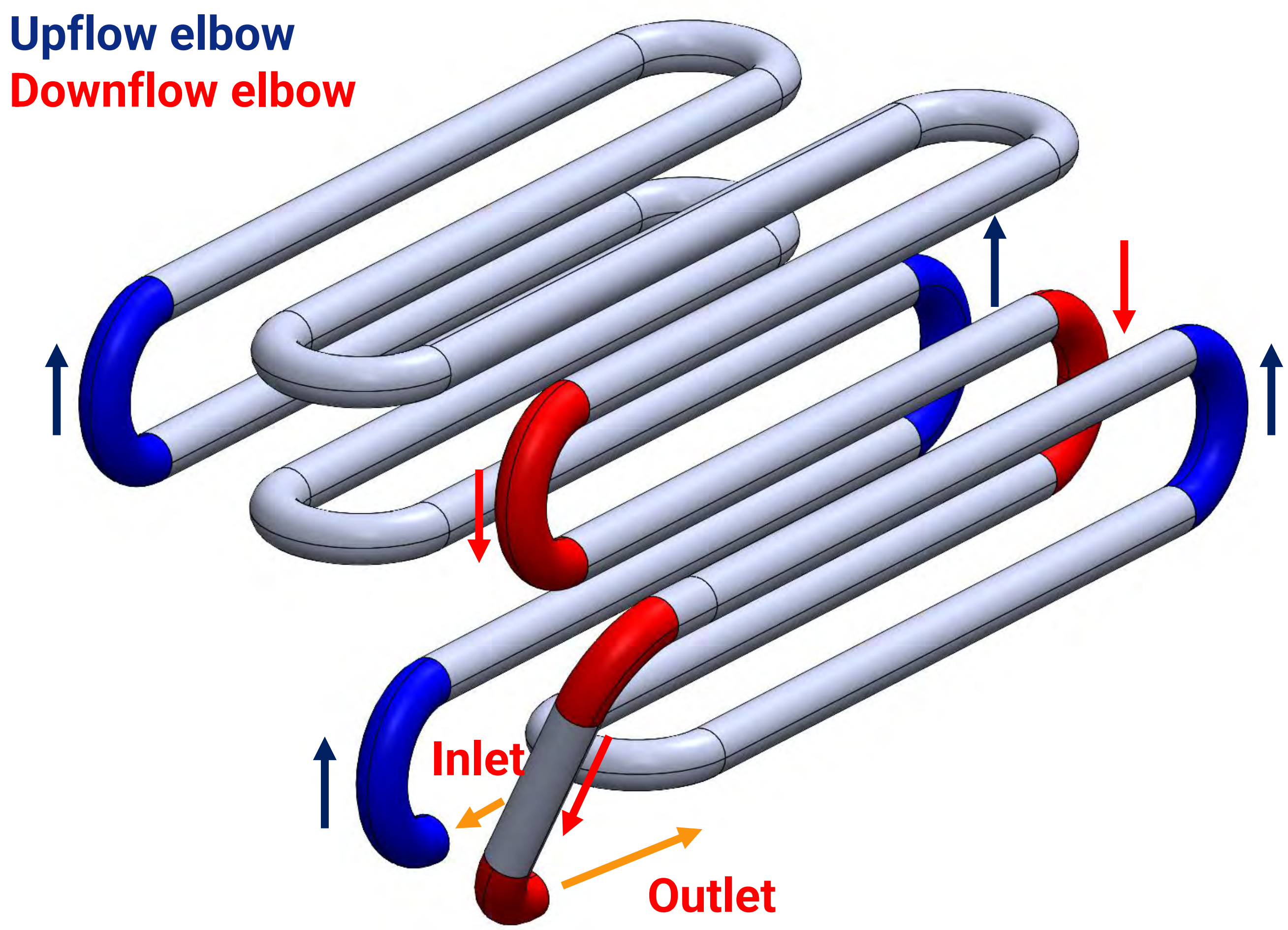
0.218%

- Whether the HT is flat or sloped upward, there is marginal difference from the flow uniformity
- Sloped HT does have longer residence time compared with float one from the torsional flow turning (out-of-plane)

What about air entrapment in the HT?

An existing HT (inside the box) outside US

Air entrapment is unlikely to happen in flat or sloped HT, then under which configuration it may happen?



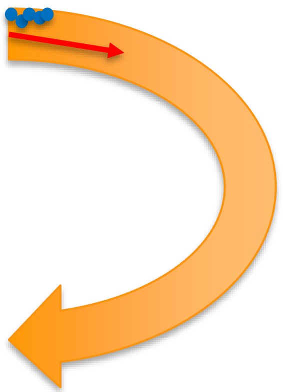
Multiple scenarios on this HT were analyzed using modeling.

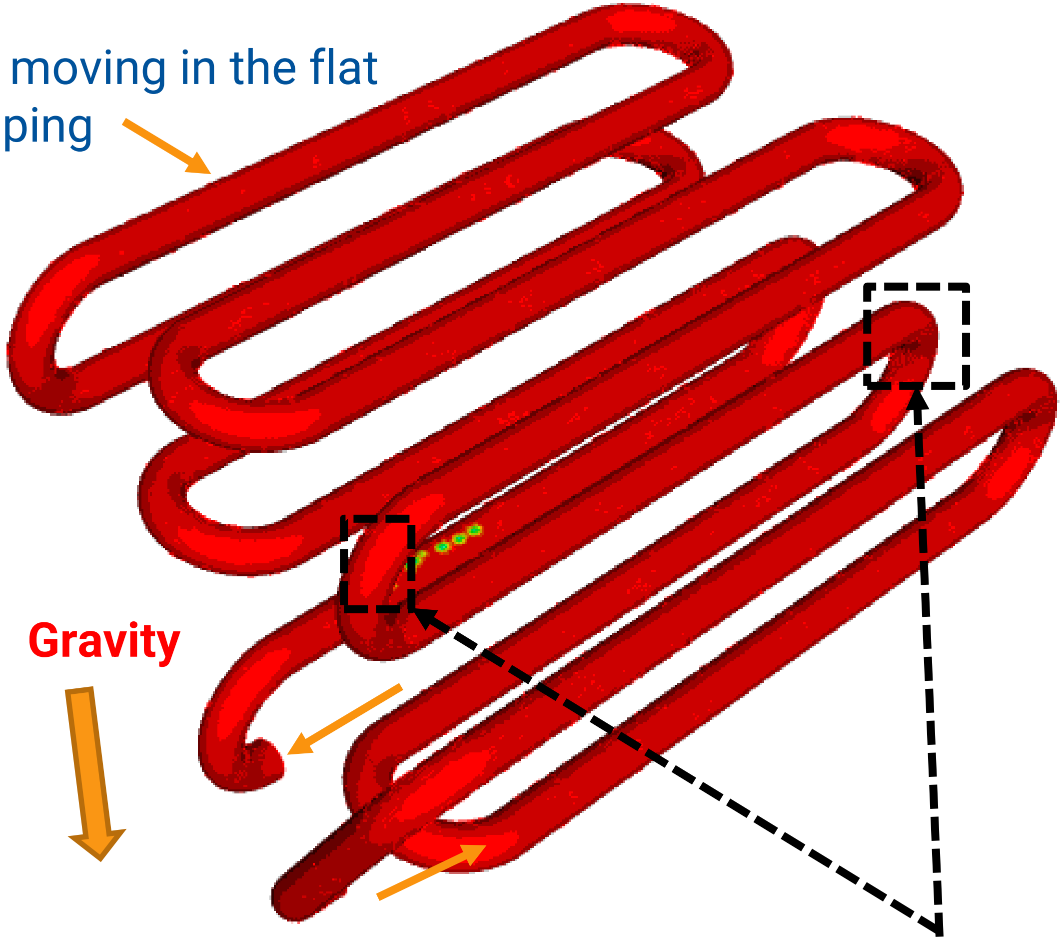
- It does provide comparable holding time to the flat and sloped one for a given length.
- Air entrapment is identified in several downflow elbow regions

An existing HT (inside the box) outside US

Air bubbles are moving in the flat portion, no trapping

Small air bubbles coalesce into larger bubble, larger buoyancy force, reduce effective flow path so flow locally accelerates





Air bubble tend to trap at downturns

- Air entrapment does happen at downturns (downflow elbow) of the HT
- Up to 4 Bar back pressure on the HT does not affect the air entrapment
- Higher flowrate can help to move the entrapped air

Takeaway from this case

- Sloped HT
  - Longer residence time due to extra out-of-plane turning
- Flat HT x Slopped HT
  - Comparable flow uniformity
- Air entrapment (on an existing HT outside US)
  - Can happen with downward flow (local flow acceleration as trapped air reduce the flow path)
- HT modeling can be used for what if analysis and more learning will be generated when we use the HT model to study different scenarios (design, conditions)

Modeling and simulation has demonstrated the potential to study and optimize process, reduce the physical testing, and speed up projection execution

When the models are fully validated, virtual testing using M&S allows:

- Visualize the obvious
- Provide directional guidance

- ⬇ Physical experiments
- ⬇ Required microbial challenge test (Combined with sanitizer kill effect)
- ⬆ Project execution speed, better and faster decision making

Question?

Acknowledgement

My colleagues in PepsiCo:

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Yuqian Lou, Process Authority

Fernanda Michelutti, Process Authority

*Amy Huchthausen, SC Eng Sr Project Manager

Advait Bhat, R&D Pkg Principal Engineer

Lei Zhao, R&D Ana Tech Director