POSTER 5

# Using Machine Learning to Predict Residence Time Distributions in Coiled Flow Inverter (CFI) Reactors

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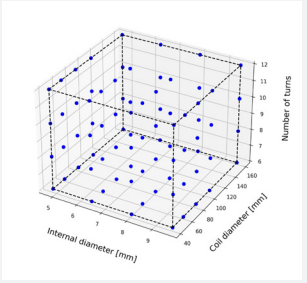
## INTRODUCTION

- A CFI reactor consist of a inner tube wrapped around a circular frame. This geometry leads to the formation of secondary flow patterns (Dean vortices) known to improve radial mixing.
- Better radial mixing results in a tighter residence time distribution ($RTD$). Many processes, such as virus inactivation, require a tight $RTD$ to avoid unwanted transformations or product damage.
- The tightness of the $RTD$ can be evaluated using the relative width ($R_w$), the ratio between the minimum and maximum residence times. An $R_w$ value of 1 corresponds to an ideal plug flow reactor.

## DESIGN OF EXPERIMENTS




- The DoE was based on an specific case study provided by our industrial partner.
- Fluid properties: $\mu$ = 0.003474 kg/m/s and $\rho$ = 966 kg/m³. | Flowrate = 22 ml/min.
- A full factorial design was carried out by varying the internal diameter ($D_i$), coil diameter ($D_c$) and number of turns. The pitch was set to 1.5 times $D_i$.
- Each point in the DoE cube was also studied at a flowrate of 66 ml/min to explore $R_w$ values at larger Reynolds numbers ($Re$), where:

$$Re = \frac{u\ D_i\ \rho}{\mu}$$

$u$: Flow velocity

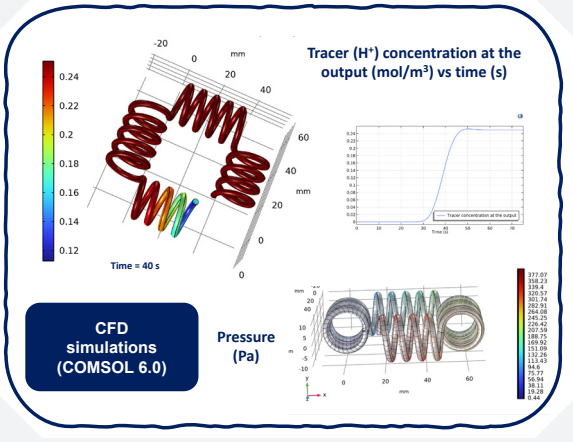
## SCALING DOWN APPROACH

- The reactors in the DoE were scaled down to a volume of 10 ml to reduce computational time and facilitate their manufacture using a 3D printer.
- The flowrate and the CFI's geometrical parameters ($D_i$, $D_c$ and pitch) were multiplied by the same scaling factor. → Reynolds number remained constant.
- CFD simulations were run for 3 full-size reactors and their corresponding scaled-down counterparts. Computational time was reduced by 80 % (~ 9.5 hours) for the largest of the 3 reactors.

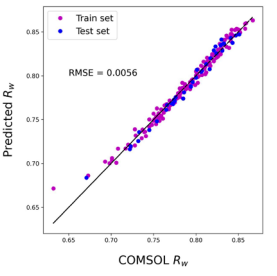
*Table 1. Correlations between full-size reactors (subscript 1) and scaled-down reactors (subscript 2) for the volume (V), pressure drop (ΔP), mean residence time ($\bar{\tau}$) and $R_w$. The scaling factor is represented with sf.*

| Volume | $\Delta P$ | $\bar{\tau}$ | $R_w$ |
|---|---|---|---|
| $V_2 = V_1\ x\ sf^3$ | $\Delta P_2 = \frac{\Delta P_1}{sf^2}$ | $\bar{\tau}_2 = \bar{\tau}_1\ x\ sf^2$ | $R_{w2} = R_{w1}$ |

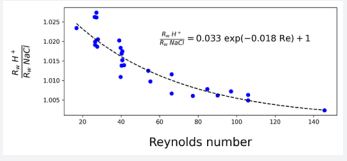
Simulated $R_w$ values from 190 4-coils reactors obtained using the transport of diluted species module in COMSOL were used to train a multivariate adaptive regression splines (MARS) model. The model's input parameters were: Reynolds number, $D_c/D_i$ and number of turns.




## $R_W$ METAMODEL (MM)



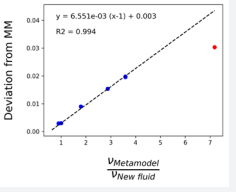

## USING NaCl AS TRACER



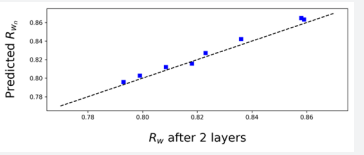

- Ratio between $R_w$ values obtained using H⁺ as the tracer and the values obtained when running the same simulations with a different tracer: NaCl.
- Both tracers had the same concentration and only differed on their diffusion constant.

## USING OTHER FLUIDS

RMSE of the values predicted by the metamodel with respect to CFD data as a function of the ratio between the kinematic viscosity of the fluid used to train the metamodel ($\nu = 3.6\ 10^{-6}$ m²/s) and the new fluid's kinematic viscosity.




## MULTILAYER




Equation for $R_w$ after n layers

$$R_{w_n} = \frac{n - \sqrt{n}\ \frac{(1-R_w)}{(1+R_w)}}{n + \sqrt{n}\ \frac{(1-R_w)}{(1+R_w)}}$$

## CONCLUSIONS

- Using a scaled-down approach to simulate industrial reactors reduces computational time and power without loss in accuracy.
- A mathematical model can be used to predict $R_w$ values of CFI reactors without having to run CFD simulations, which are not always straight forward and usually require the use of a high-performance computer.
- $R_w$ values depend on the fluid and tracer used in the simulation, nonetheless this effect can be accounted for and included in the metamodel.