Modeling Flow and Residence Time Distribution (RTD) in an Industrial-scale Segmented Reactor by Coupling CFD and Monte Carlo Simulations

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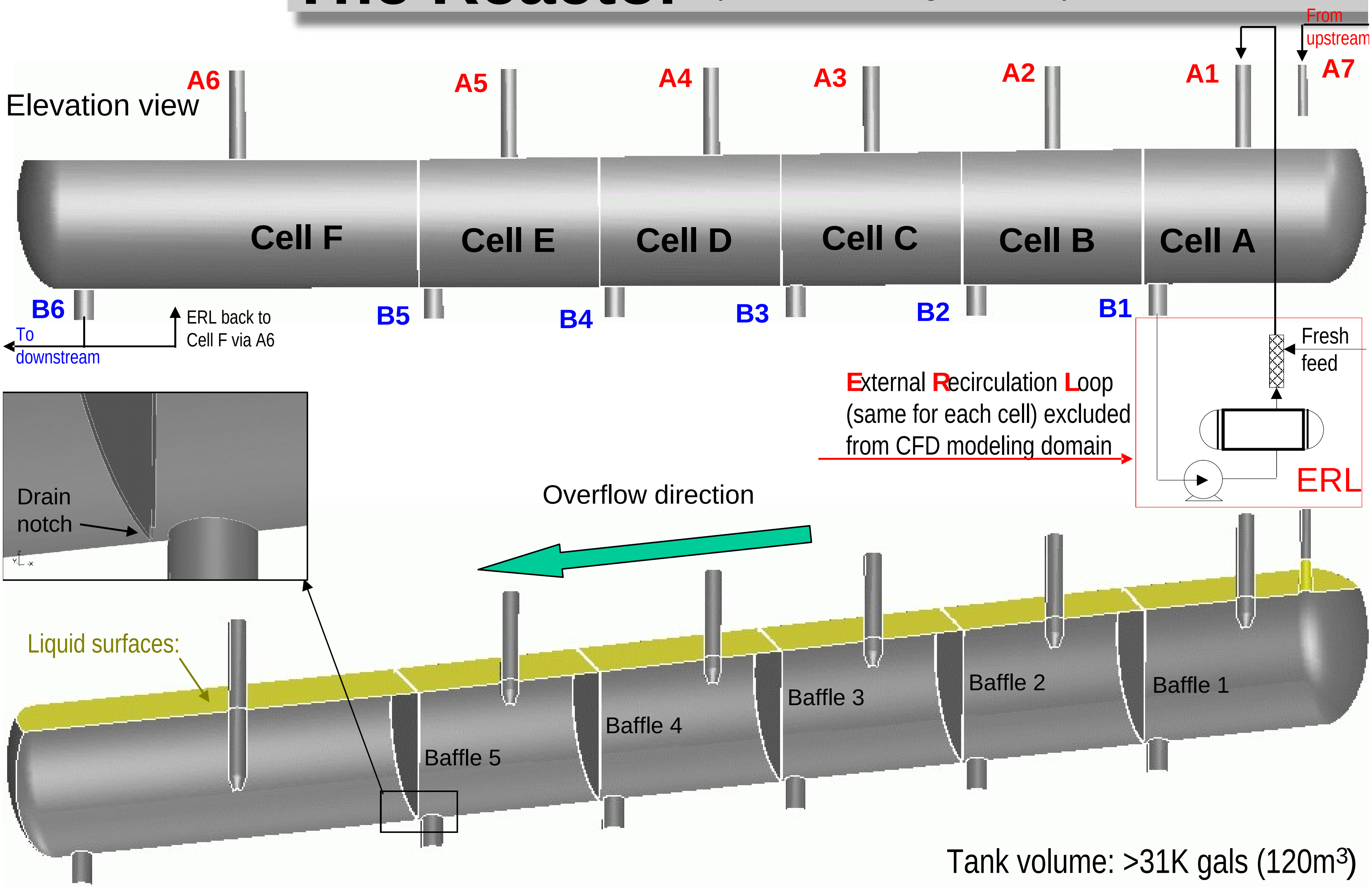
The Dow Chemical Company

Introduction

- Motivation
- Quantifying flow and RTD in a reactor is critical for defining appropriate reactor model to predict performance (e.g., yield and selectivity)
  - What reactor model to use (CSTR, PFR or combination)
  - Process optimization
  - Evaluation of different operating conditions
- This talk: RTD

The Reactor (CFD modeling domain)

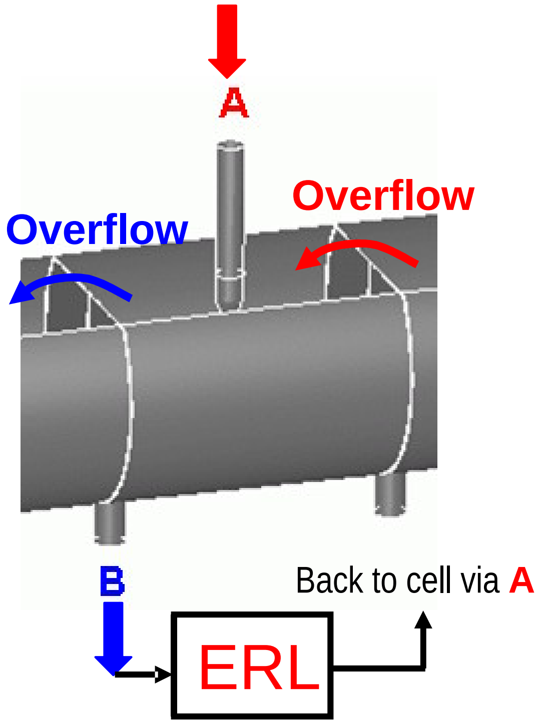


RTD Strategy

- *Measuring* RTD in the reactor during operation is expensive and difficult
  - Lab experiment scale-up is difficult
- *Modeling:* "2-step" approach
  - Step 1: obtain the flow field in the reactor (frozen in Step 2)
  - Step 2: obtain RTD (2 methods)
    - Method 1: Predict the outlet response to a pulse or step input at the inlet (transient simulation of passive scalar)
    - Method 2: Stochastic particle tracking to track trajectories of tracers (statistically calculate RTD)
      - Tracers released at inlets of each cell
      - Random Walk Model for dispersion due to turbulent eddies
      - Residence time recorded @ outlets as each tracer exits the cell
    - Method 2 chosen in this work
      - Advantage in dealing with multiple inlets/outlets
      - Advantage in coupling with Monte Carlo method

Unique Challenges

- Multiple inlets/outlets
- External Recirculation Loop (ERL), which is excluded from the CFD modeling domain

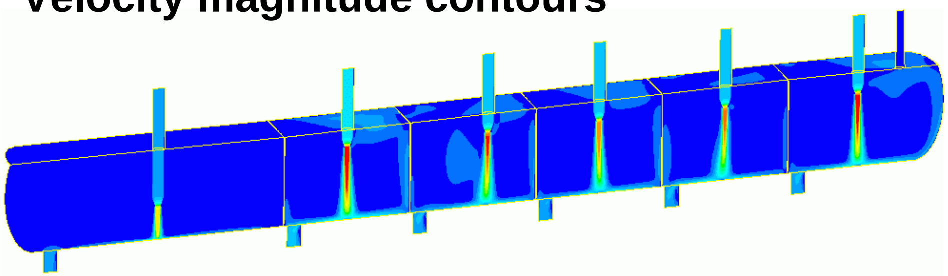


Cell RTD components without **ERL**

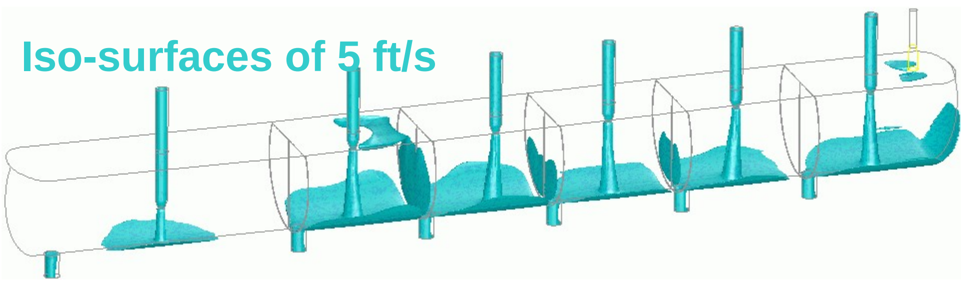
Cell RTD	Tracers released @:	Tracers exiting cell @: (where RT recorded)
RTD_{OO}	Overflow from previous cell	Overflow to next cell
RTD_{OB}	Overflow from previous cell	Outflow via nozzle B
RTD_{AO}	Inflow via nozzle A	Overflow to next cell
RTD_{AB}	Inflow via nozzle A	Outflow via nozzle B

Flow Patterns

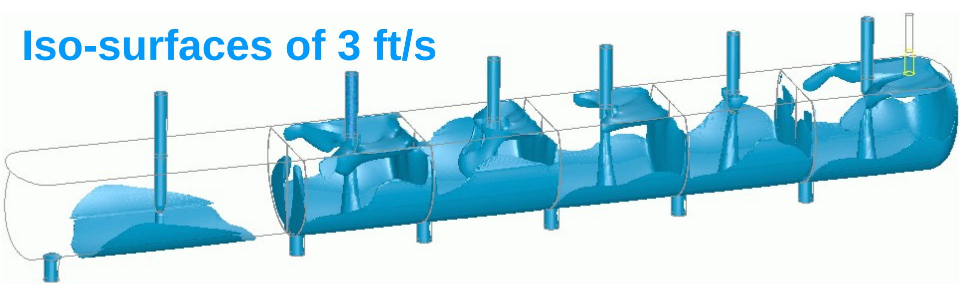
Velocity magnitude contours



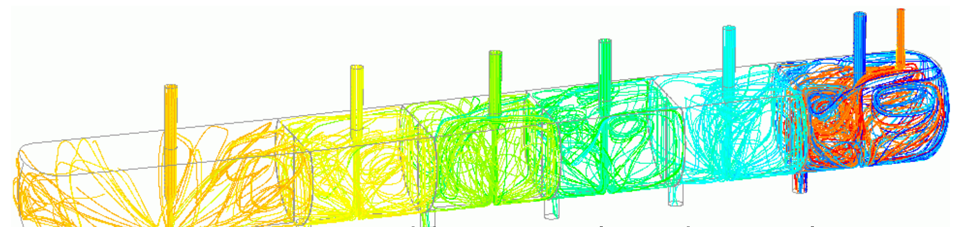
Iso-surfaces of 5 ft/s



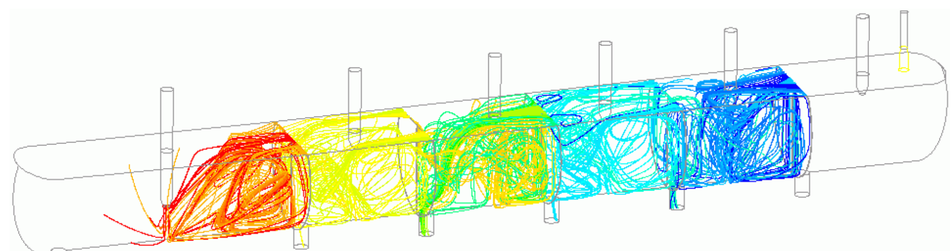
Iso-surfaces of 3 ft/s



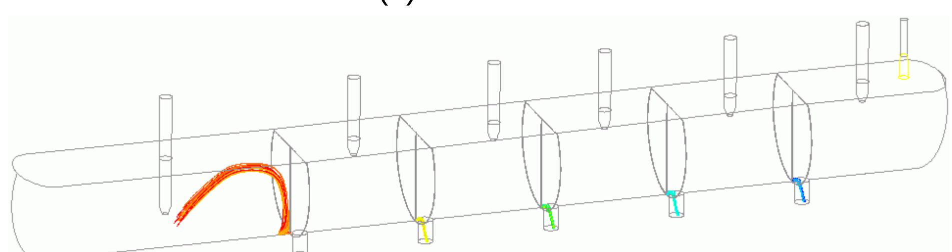
Flow pathlines:



(a) Tracers released at Nozzle A1-A7



(b) Tracers released at baffle overflows



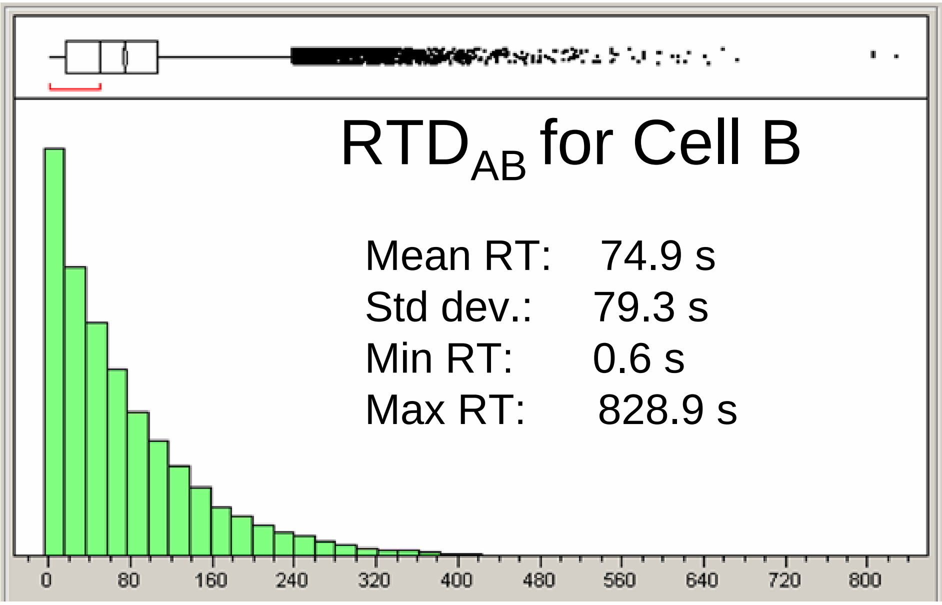
(c) Tracers released at drain notches

FLUENT 6.3

RTD components w/o ERL

Key elements for accurate stochastic tracer tracking

- -- Tracer release distribution @ inlets based on local mass flow rate
- -- Sufficient number tracers tracked to produce statistically significant results
- Average 35,000 tracers tracked in each stochastic tracking
- -- Proper integration time step



"How to" in FLUENT

Tedious "Inlet subdivisions" approach

- Divide inlet into multiple sub-inlets based on velocity range
- Define "Injection" for *each* sub-inlet
  → # tracers ~ local mass flow rate

Validation of RTD w/o ERL

$$t_C = \frac{V}{Q_T}$$

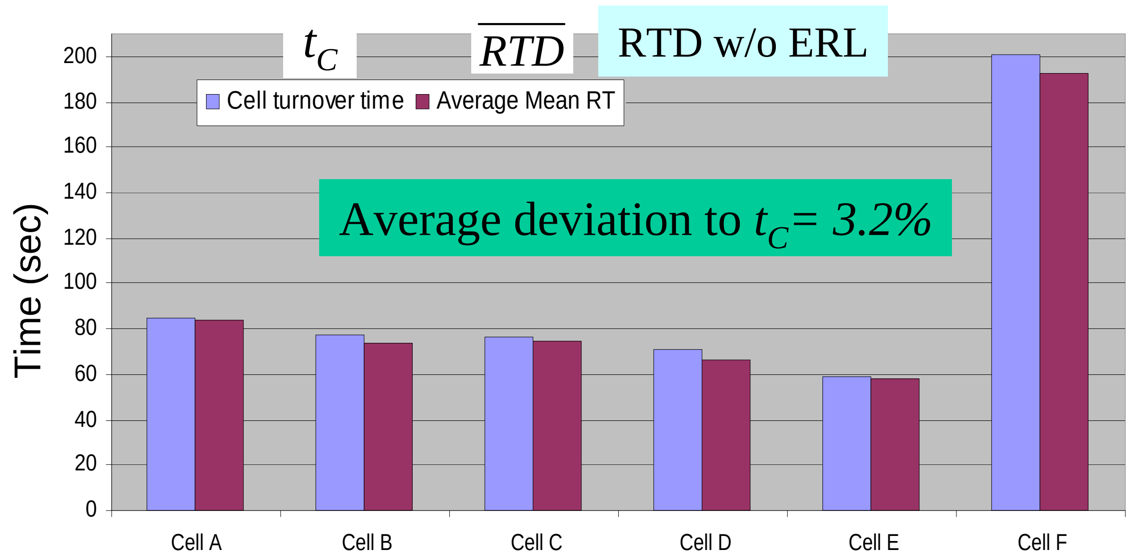
$$\overline{RTD} = \beta\left(\psi_{OO}\overline{RTD_{OO}} + \psi_{OB}\overline{RTD_{OB}}\right) + (1-\beta)\left(\psi_{AO}\overline{RTD_{AO}} + \psi_{AB}\overline{RTD_{AB}}\right)$$

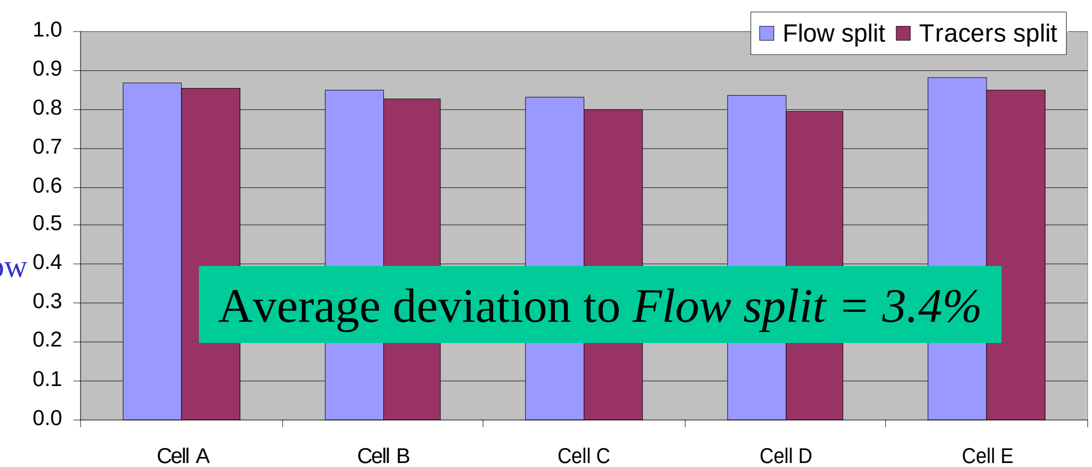
(Ave. weighted by tracer split *and* inflows)

$\beta = \frac{Q_O}{Q_T}$ Ratio of weir overflow in inflows

$\overline{RTD_{OO}}$ Mean RT for RTD_{OO}

ψ_{OO} Tracer-split ratio in tracking



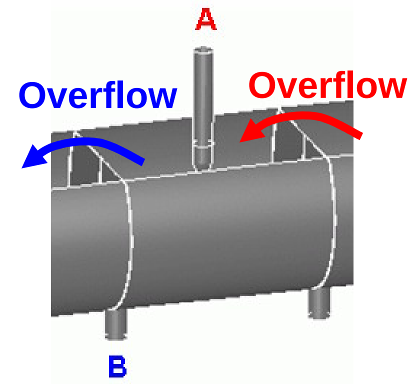


Flow split (C): ratio of flow being recycled and total inflow

Tracers split: ratio of tracers exiting Nozzle B and total injected tracers

Include ERL in RTD

- Key information
  - Single-pass RTDs for each cell: RTD_{OO}, RTD_{OB}, RTD_{AO}, and RTD_{AB}
  - C – (flow recycled back to the cell) / (total inflow entering the cell)
  - Δt – lag time through **ERL**



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Cycles experienced	% tracers being tracked	RTD with effect of flow recycling
0	$(1-C)$	RTD_{OO}
1	$(1-C)C$	$RTD_{OB} + \Delta t + RTD_{AO}$
2	$(1-C)C^2$	$RTD_{OB} + RTD_{AB} + 2\Delta t + RTD_{AO}$
3	$(1-C)C^3$	$RTD_{OB} + 2RTD_{AB} + 3\Delta t + RTD_{AO}$
…	…………	………………
n	$(1-C)C^n$	$RTD_{OB} + (n-1)RTD_{AB} + n\Delta t + RTD_{AO}$

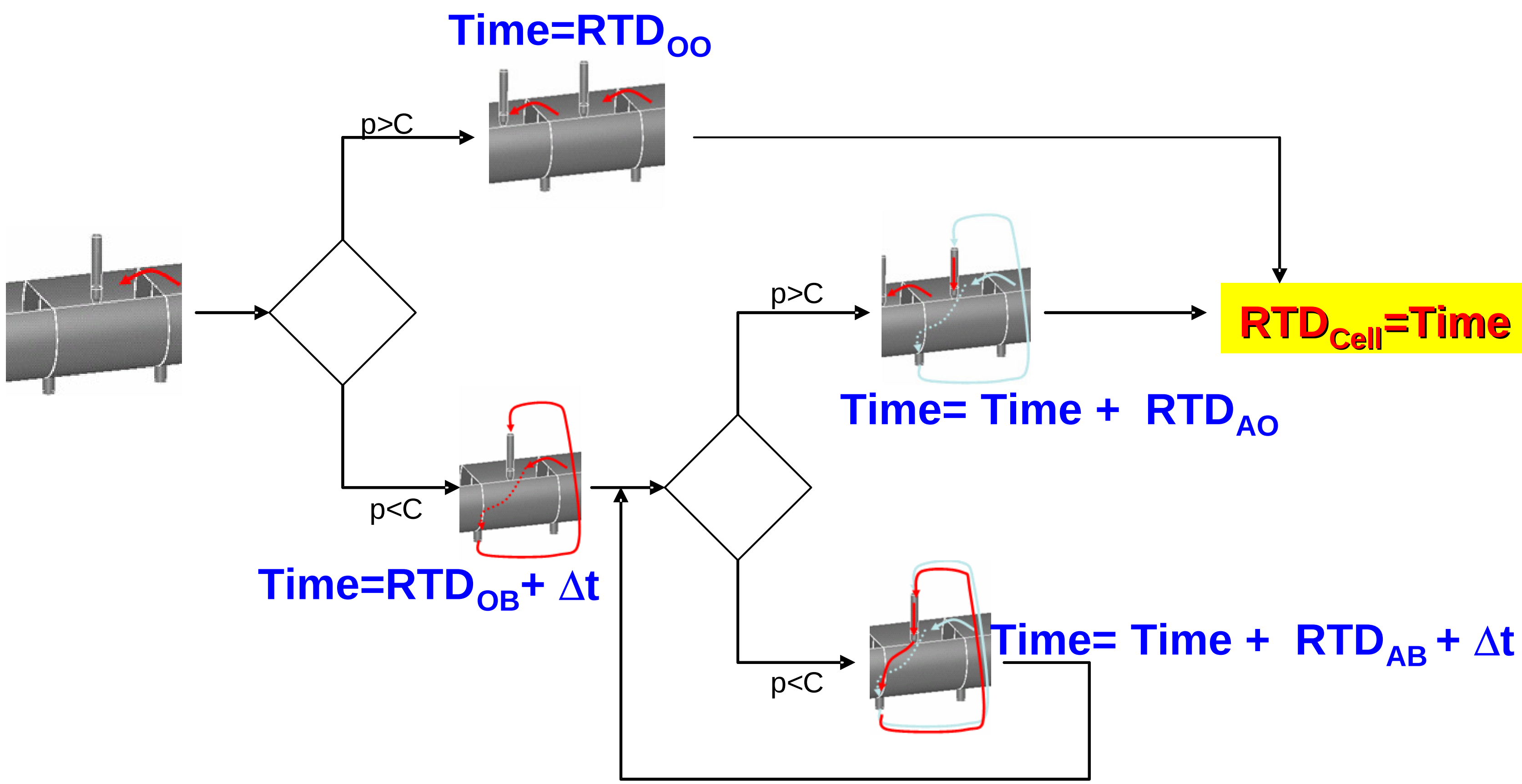
Number of cycles (n) needed to track all tracers

$$(1-C) + (1-C)C + (1-C)C^2 + (1-C)C^3 + \ldots + (1-C)C^n = 1$$

for example, if C=0.9, 99% tracers would be tracked after 43 cycles (n =43)

- "+" operations between the single-pass RTDs (raw data) → superposition through Monte Carlo simulation

Monte Carlo Schematic

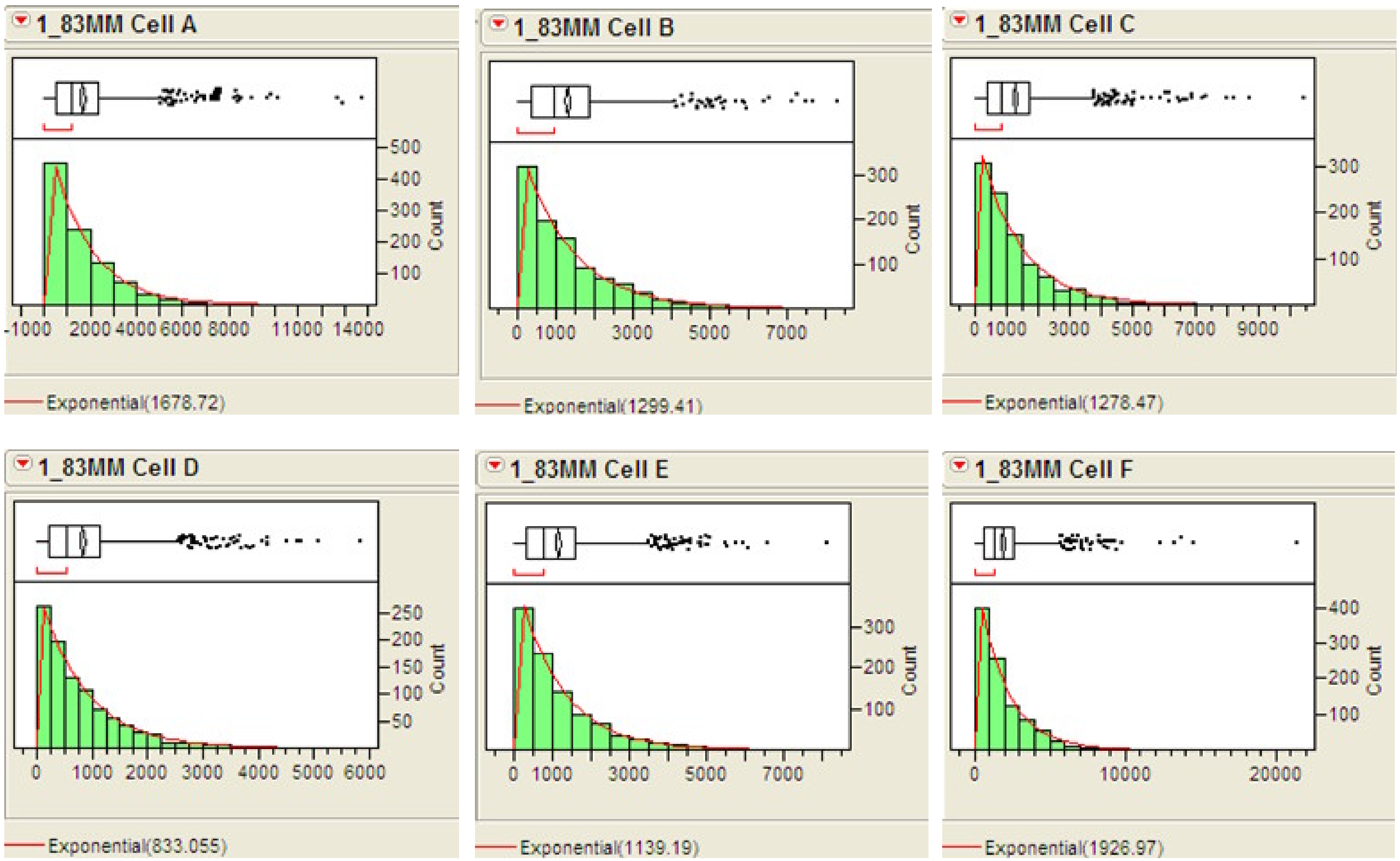


p – random number, uniformly distributed between 0 and 1

C – (flow recycled back to the cell) / (total inflow entering the cell)

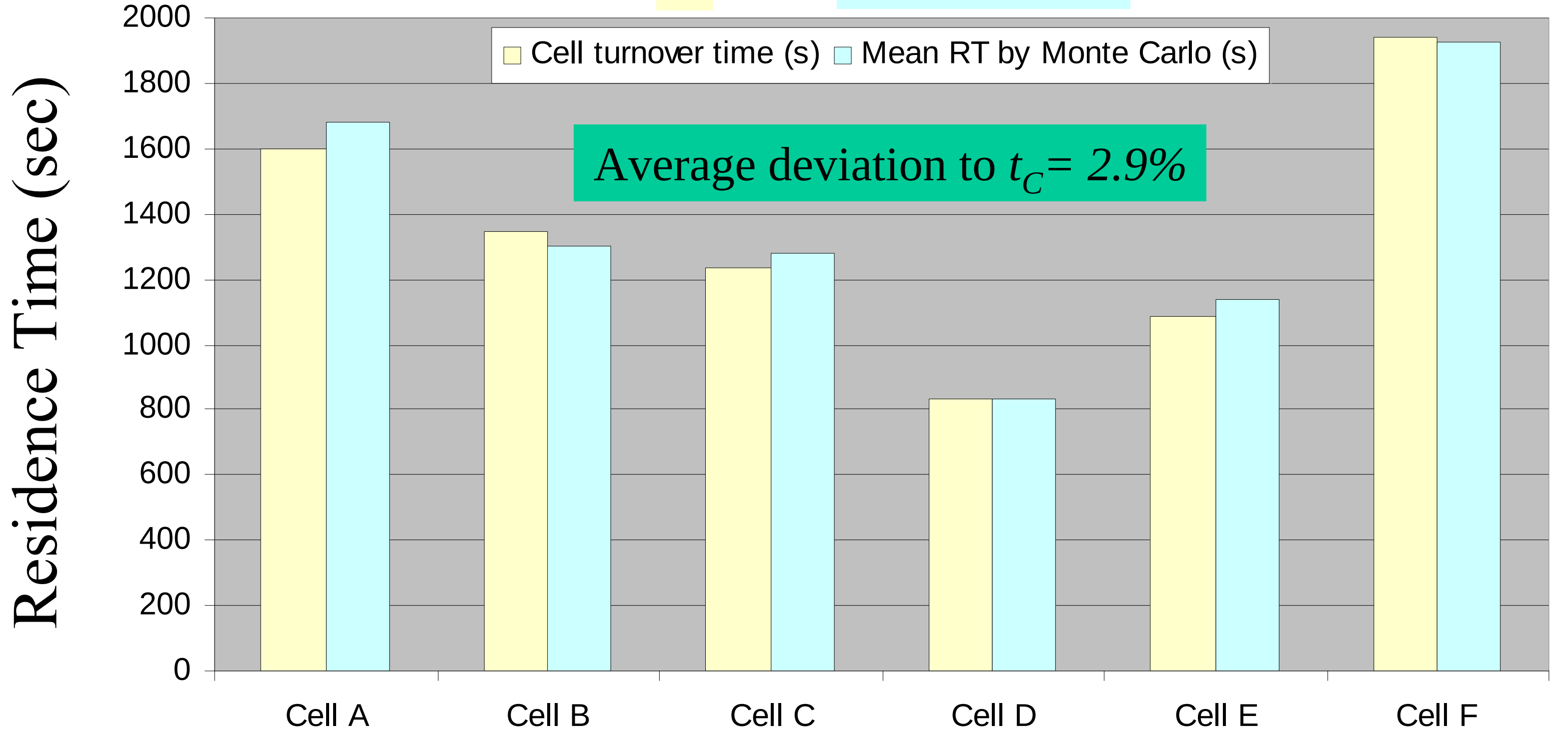
Monte Carlo simulation using the commercial software ARENA by Rockwell Automation Technologies Inc.

Histograms of RTD w/ERL



Validation of RTD w/ERL

t_C RTD w/**ERL** **ERL**: **E**xternal **R**ecirculation **L**oop



Cell turnover time: $t_C = \frac{V'}{Q'_T}$

V' = the liquid volume in the cell + in the ERL

Q'_T = (the total volumetric flow rate entering the cell) - (the flow being recycled back to the cell)

Summary

- A model was developed to predict RTD in a reactor with multiple inlets and outlets as well as external recirculation loop (ERL)
  - by coupling CFD stochastic particle tracking with Monte Carlo simulation (implemented in ARENA by Rockwell Automation Technologies Inc.)
  - validated by matching the reactor/cell turnover times
    - also by matching “flow split” with “tracers split”
- Critical for accurate RTD predictions during stochastic particle tracking
  - Tracer release distribution @ inlets proportional to local mass flow rate
  - Sufficient number of tracers tracked to produce statistically significant results
  - Proper integration time step

Thank You