Flow characteristics in flow battery

AVIK GHOSH

Problem Statement:

- Determination of stagnant zone/ dead volume in flow compartments

{Lesser dead volume} → {Small residence time for electrolyte} → {Increment in reaction efficiency}

- **APPROACHES:**

VELOCITY FIELD

1. Determine the flow field
2. Identify low velocity zone

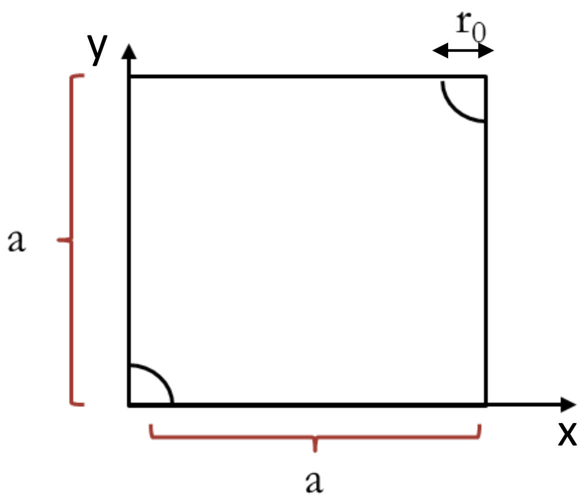
RTD

1. Determination of residence time distribution curve
2. Calculate the area under tail of the curve (> t_1)
3. Quantify dead volume

2D – Flow Field:

Assumptions:

- Ideal, incompressible Fluid
- Diagonally opposite inlet & outlet
- $V_r(r)$ is the only non-zero velocity component



Governing equation & B.C:

$$\nabla \cdot \mathbf{v} = 0$$

- Velocity at $r = r_0$ is U_0

Solution for inlet:

$$v_r = \frac{U_0 r_0}{r}$$

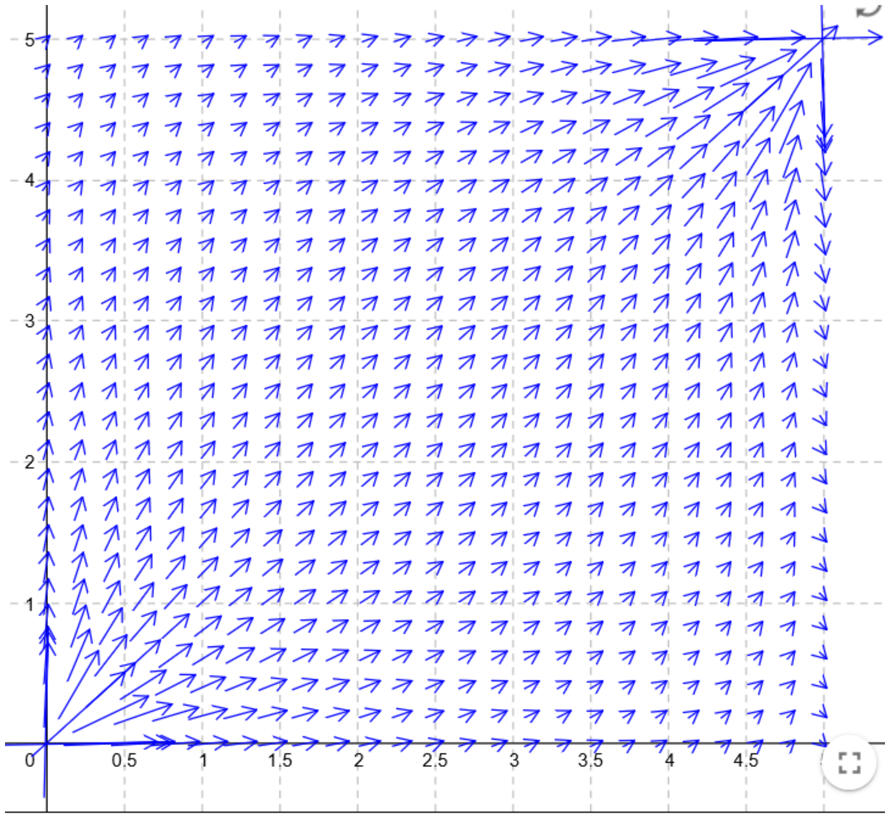
Solution for outlet:

$$v_r = -\frac{U_0}{r}\left(\frac{r_0^2 - a^2}{2a} + r\cos(\theta)\right)$$

Velocity Profile:

Total velocity as a function of r and θ:

$$v_r = \frac{U_0 r_0}{r} - \frac{U_0}{r}\left(\frac{r_0^2 - a^2}{2a} + r\cos(\theta)\right)$$



Plotted with wolfram

2D- Flow Profile for Viscous fluid:

Assumptions:

- Incompressible, Newtonian, steady-state

Governing Equations:

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\left(\frac{1}{\rho}\right)\frac{\partial p}{\partial x}+\nu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right),$$

$$u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\left(\frac{1}{\rho}\right)\frac{\partial p}{\partial y}+\nu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right),$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0.$$

Non-dimensionalization $\longrightarrow$

$$u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{\partial p}{\partial x}+\left(\frac{1}{\mathrm{Re}}\right)\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right),$$

$$u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{\partial p}{\partial y}+\left(\frac{1}{\mathrm{Re}}\right)\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right),$$

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0,$$

Here, $u \to u/U_0,\ v \to v/U_0,\ p \to p/(\rho U_0^2),\ x \to x/L,\ y \to y/L,$

And $\mathrm{Re} = \frac{\nu L}{U_0}$

RTD for 2D flow:

Governing equation(convection-diffusion equation):

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right)$$

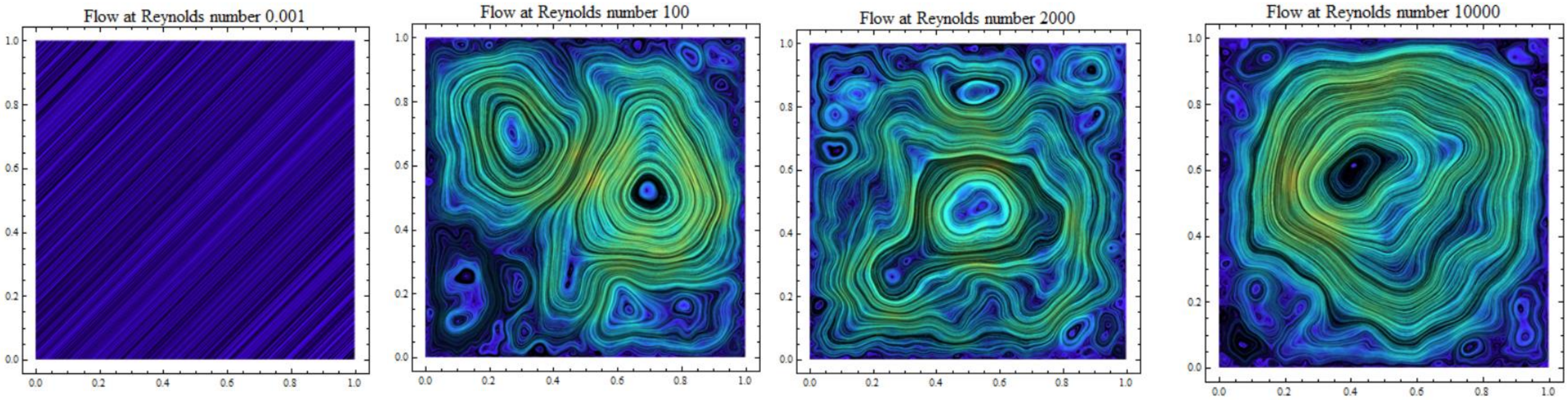
After non-dimensionalization:

$$\bar{x} = \frac{x}{L}, \quad \bar{y} = \frac{y}{L}, \quad \bar{t} = \frac{t}{T}, \quad \bar{C} = \frac{C}{C_0}$$

Pe = uT/L, Sc = ν/D

$$\boxed{\frac{\partial \bar{C}}{\partial \bar{t}} + Pe\frac{\partial \bar{C}}{\partial \bar{x}} + Pe\frac{\partial \bar{C}}{\partial \bar{y}} = \frac{1}{Sc}\left(\frac{\partial^2 \bar{C}}{\partial \bar{x}^2} + \frac{\partial^2 \bar{C}}{\partial \bar{y}^2}\right)}$$

2D flow profile:



3D Case:

Algorithm:

CFD flow field → Particle tracer → RTD curve → Quantification of Dead Volume

Parameters:

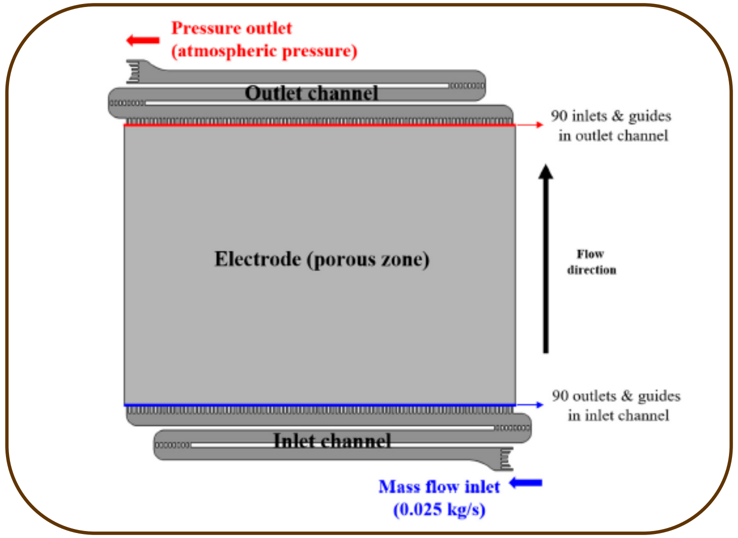
1. Geometry 2. Flow rate

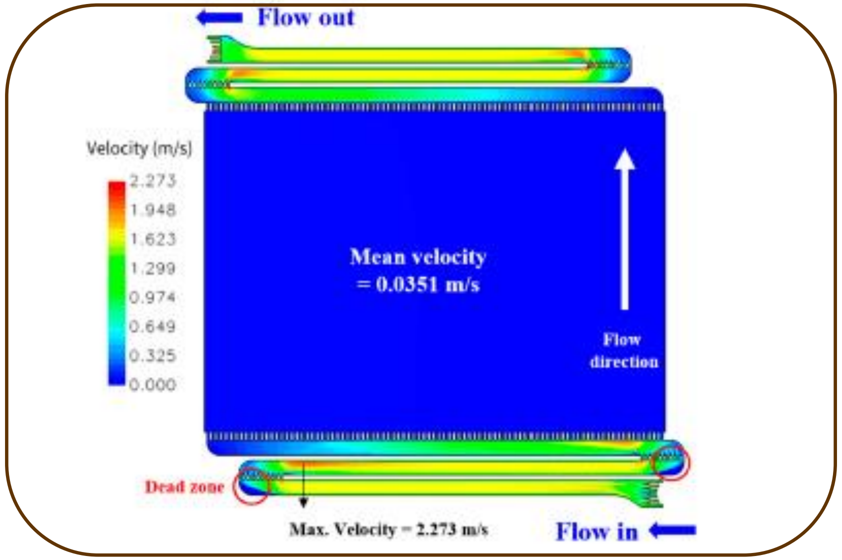
Design:

Reduction of dead volume:

- Reduction of formation of eddies at corners
- Uniform flow

Jun-Yong Park et.al, 2020





CODES:

```
In[297]:= opt = "DifferenceOrder" → 4;
dfdx = NDSolve`FiniteDifferenceDerivative[{1, 0},
    {nx, nx}, opt]["DifferentiationMatrix"];
dfdy = NDSolve`FiniteDifferenceDerivative[{0, 1},
    {nx, nx}, opt]["DifferentiationMatrix"];
d2fdx2 = NDSolve`FiniteDifferenceDerivative[{2, 0},
    {nx, nx}, opt]["DifferentiationMatrix"];
d2fdy2 = NDSolve`FiniteDifferenceDerivative[{0, 2},
    {nx, nx}, opt]["DifferentiationMatrix"];

Rey = 0.0001;
eqnsU = varsU * (dfdx.varsU) + varsV * (dfdy.varsU) + dfdx.varsP - (1/Rey) * ((d2fdx2 + d2fdy2).varsU);
eqnsV = varsU * (dfdx.varsV) + varsV * (dfdy.varsV) + dfdy.varsP - (1/Rey) * ((d2fdx2 + d2fdy2).varsV);
eqnsCont = dfdx.varsU + dfdy.varsV;
```

```
In[302]:= boundaries = Union[Flatten[Position[grid, #] & /@ {{0., _}, {1., _}, {_, 0.}, {_, 1.}}]];
topBndry = Flatten@Position[grid, {1, 1}];
bottomBndry = Flatten@Position[grid, {0, 0}];
bndryComp = Complement[boundaries, topBndry];

eqnsU[[boundaries]] = varsU[[boundaries]];
eqnsU[[topBndry]] = varsU[[topBndry]] - 1;
eqnsU[[bottomBndry]] = varsU[[bottomBndry]] - 1;
eqnsV[[boundaries]] = varsV[[boundaries]];
eqnsV[[topBndry]] = varsV[[topBndry]] - 1;
eqnsV[[bottomBndry]] = varsV[[bottomBndry]] - 1;
eqnsCont[[topBndry[[1]]]] = varsP[[topBndry[[1]]]];
eqnsCont[[bottomBndry[[1]]]] = varsP[[bottomBndry[[1]]]];
Part::partw : Part 1 of {} does not exist. >>
Part::pspec : Part specification {}[[1]] is neither a machine-sized integer nor a list of machine-sized integers. >>
Part::partw : Part 1 of {} does not exist. >>
Set::pspec : Part specification {}[[1]] is neither a machine-sized integer nor a list of machine-sized integers. >>
```

```
In[273]:= govExpr = Join[eqnsU, eqnsV, eqnsCont];
allVars = Join[varsU, varsV, varsP];

Length /@ {govExpr, allVars}
Out[275]= {30000, 30000}

In[206]:= {30000, 30000}
Out[206]= {30000, 30000}

In[276]:= sol = allVars /. FindRoot[govExpr, Thread[{allVars, 1}]];
FindRoot::lstol : The line search decreased the step size to within tolerance specified by Accurac
FindRoot::lstol : The line search decreased the step size to within tolerance specified by Accuracy
FindRoot::lstol : The line search decreased the step size to within tolerance specified by Accuracy
FindRoot::lstol : The line search decreased the step size to within tolerance specified by Accuracy
```

```
In[306]:= {usoltemp, vsoltemp, psoltemp} = Partition[sol, nL];
usol = Interpolation@ Join[grid, Transpose@List@usoltemp, 2];
vsol = Interpolation@ Join[grid, Transpose@List@vsoltemp, 2];
psol = Interpolation@ Join[grid, Transpose@List@psoltemp, 2];

In[311]:= LineIntegralConvolutionPlot[{{usol[x, y], vsol[x, y]}, {"noise", 1000, 1000}},
  {x, 0, 1}, {y, 0, 1}, LineIntegralConvolutionScale → 3,
  ColorFunction → "BlueGreenYellow",
  PlotLabel → Style[Text["Flow at Reynolds number 0.001"], 18]]
```

References:

1. Skyllas-Kazacos M, Chakrabarti MH, Hajimolana SA, Mjalli FS, Saleem M. Progress in flow battery research and development. *J Electrochem Soc*. 2011; 158(8): R55-R79
2. Macdonald, Malcolm, and Robert M. Darling. "Comparing velocities and pressures in redox flow batteries with interdigitated and serpentine channels." *AIChE Journal* 65.5 (2019): e16553.
3. MacDonald, M. and Darling, R.M., 2018. Modeling flow distribution and pressure drop in redox flow batteries. *AIChE Journal*, *64*(10), pp.3746-3755.
4. Kim, Bo-Ra, et al. "A study on flow characteristics and flow uniformity for the efficient design of a flow frame in a redox flow battery." *Applied Sciences* 10.3 (2020): 929.
5. Park, Jun-Yong, Deok-Young Sohn, and Yun-Ho Choi. "A numerical study on the flow characteristics and flow uniformity of vanadium redox flow battery flow frame." *Applied Sciences* 10.23 (2020): 8427.