

Erosion in Components of Supercritical CO₂ Power Cycles

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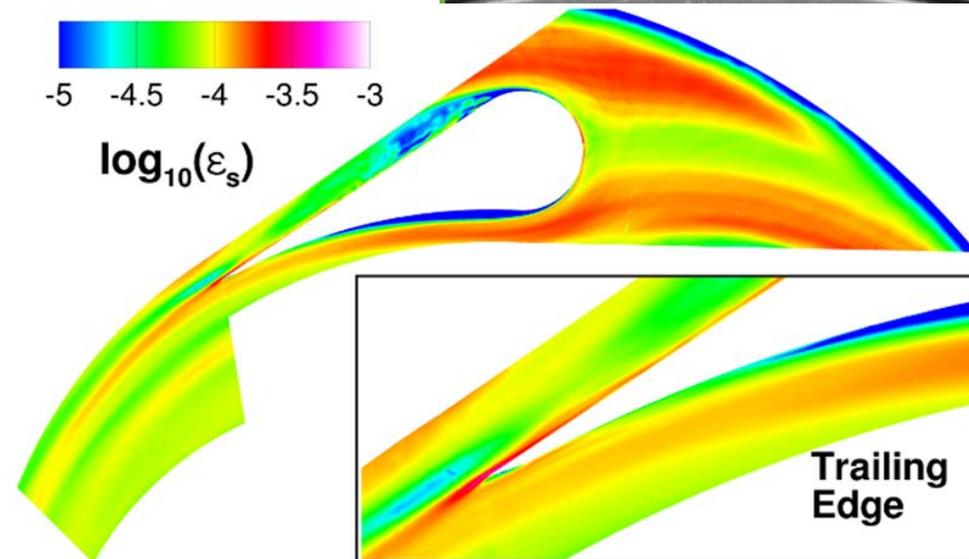
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DISCLAIMER

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Why supercritical CO₂ power cycles?

Higher Efficiency

High working fluid temperatures

Recompression near liquid densities

High heat recuperation

Lower Capital Cost

Compact turbo machinery

Simple configurations

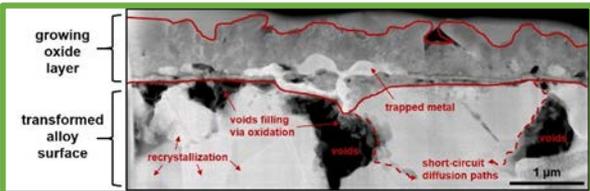
Lower Environmental Impact

Zero emissions

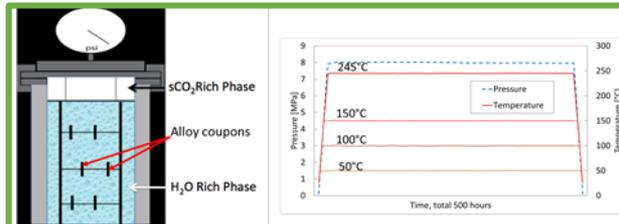
Dry cooling

Water production

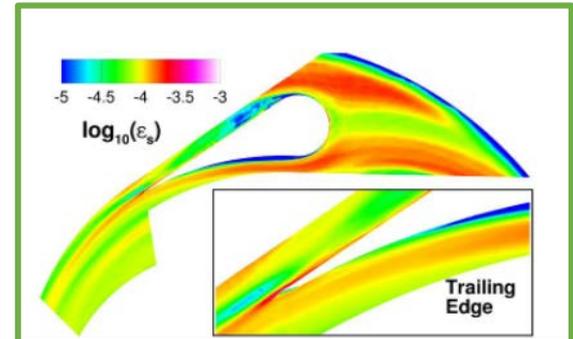
Materials Research for sCO₂ Power Cycles at NETL Research & Innovation Center



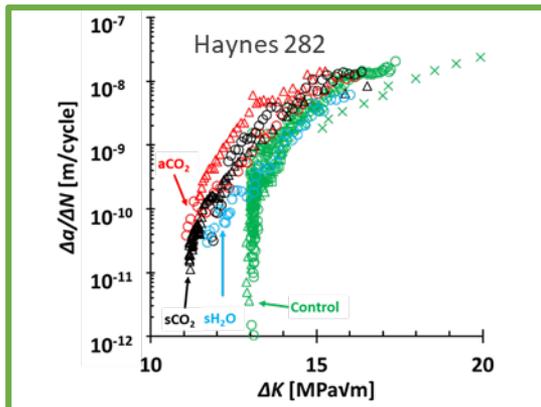
High-temperature oxidation of Ni- and Fe-based alloys in sCO₂ cycle environments



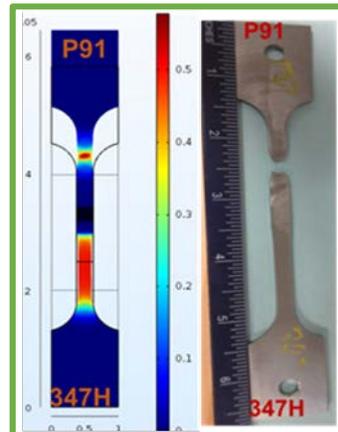
Aqueous corrosion of steels in carbonic acid environments in direct sCO₂ cycles



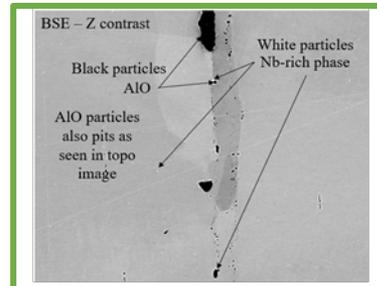
Erosion in components of sCO₂ power cycles



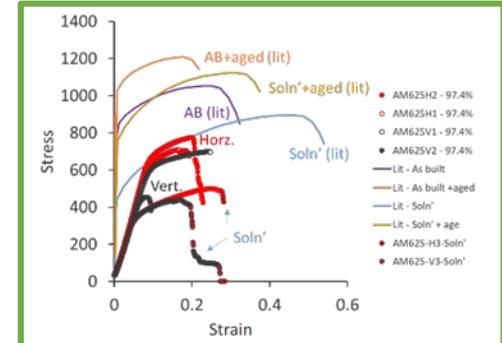
Effect of sCO₂ cycle environments on mechanical properties of high-temperature alloys



Effect of CO₂ on dissimilar metal welds



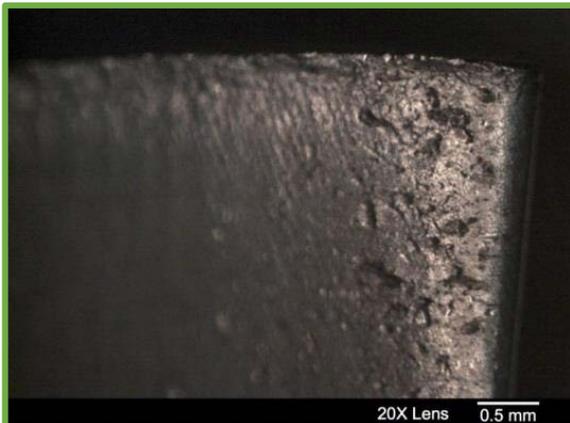
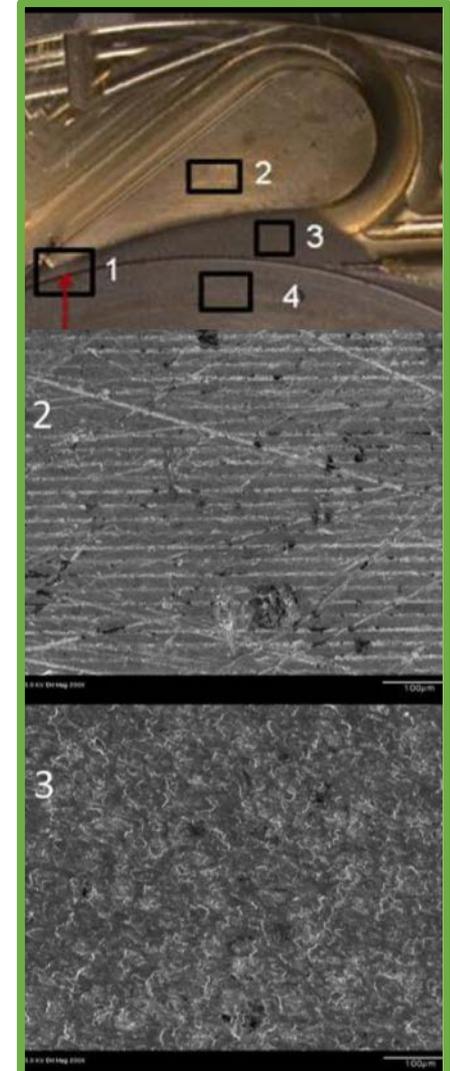
Diffusion bonding of Inconel 740H for manufacturing compact heat exchangers



Additive manufacturing of heat exchangers with gyroid geometry

Erosion in Components of sCO₂ Power Cycles

Problem: Severe erosion of turbine blades and vanes has been observed in the sCO₂ cycle test loops in Sandia National Lab and Bettis Lab.



Sandia Findings

- Particle impingement on flow surfaces
- Particles in the loop:
 - Stainless steel
 - SiO₂
 - Al₂O₃

Erosion in Components of sCO₂ Power Cycles

Our work aims to establish:

- Whether erosion might be a significant problem in sCO₂ power cycles (Is erosion a significant barrier for the commercialization of the sCO₂ power cycle technology?)
- An understanding of erosion mechanism
- A simulation tool to predict whether erosion is expected in a given turbine design
- A guidance for an experimental work which might be implemented if erosion is shown to be a problem.

Root cause of damage:

- Impact by solid particles?
- Fluctuating shear forces?
- Phase change?

Fluctuating shear forces

Hypothesis:

- Geometric orientated fluctuating shear stress may cause fatigue and erosion;

Methodology:

- To simplify the complex problem, one can, in the perspective view of fluid dynamics, take it as **turbulent flow through a pipe bend**;
- Perform **large-eddy simulations** for turbulent flows without heat transfer, at Reynolds number in a wide range from 5000 to 100,000;
- Validate the solver with available experimental and numerical data;
- Calculate the **shear stresses on the inner surface of the pipes**;
- Identify **secondary flow patterns**, such as the Dean vortices;

CFD Simulation Framework

Fluid phase (sCO₂)

- Spatially filtered, incompressible N-S for Large Eddy Simulation

$$\frac{\partial \bar{u}_j}{\partial t} + \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{1}{\rho} \frac{\partial \bar{P}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j^2} - \frac{\partial q_{ij}}{\partial x_j}$$

$\frac{\partial \bar{u}_j}{\partial x_j} = 0$

- Dynamic Smagorinsky model for SGS stress
 $q_{ij} = -2\nu_t S_{ij}$

Where,

$$\nu_t = (C_\mu \Delta)^2 |\mathbf{S}|, \quad S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

Key Assumptions

- Incompressible, low Mach number
- Constant properties (density, viscosity)
- One-way coupling (dilute assumption)

Solid phase (porous oxide particles)

- Integrate Newton's second law for individual particles.
- Total force from fluid pressure and Drag

$$\frac{d}{dt}(\mathbf{x}_p) = \mathbf{u}_p$$

$$\frac{d}{dt}(\mathbf{u}_p) = \underbrace{-\frac{1}{\rho_p} \nabla \bar{P}}_{\text{Pressure Force}} + \underbrace{\frac{f(Re_p)}{\tau_p} (\bar{\mathbf{u}} - \mathbf{u}_p)}_{\text{Drag force}}$$

Numerical Solution

- Energy conserving, co-located, finite volume discretization for arbitrary, unstructured grids¹.
- Fractional step, pressure projection time advancement.
- Fully parallelized, capable of variable density flow
- Validation for turbulent particle laden flows in complex geometries^{2,3,4}

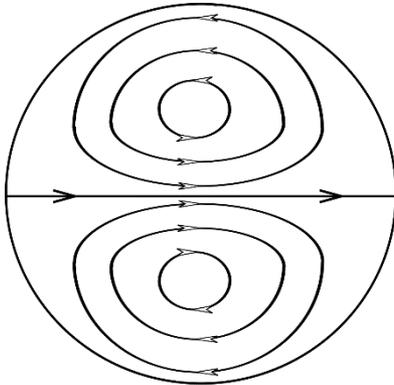
[1] Mahesh, K., Constantinescu, G., Moin, P., 2004. A numerical method for large-eddy simulation in complex geometries. J. Comp. Phys. 197, 215-240.

[2] Apte, S.V., Mahesh, K., Moin, P., Oefelein, J.C., 2003. Large-eddy simulation of swirling particle-laden flows in a coaxial-jet combustor. Int. J. Mult. Flow 29, 1311-1331.

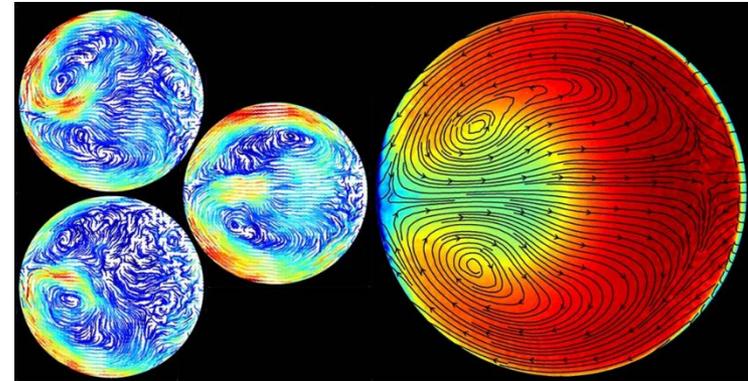
[3] Shams, E., Finn, J., Apte, S., 2011. A numerical scheme for Euler-Lagrange simulation of bubbly flows in complex systems. Int. J. for Num. Methods in Fluids 67, 1865.

Dean vortices and swirl switching

The cross flow pattern, if projected on the cross-stream plane, was identified to consist of two counter rotating vortex cells, where the flow in the center plane was directed toward the outer wall. [Dean, W. R., 1928]



(a) Dean vortices (Dean, W. R., 1928)

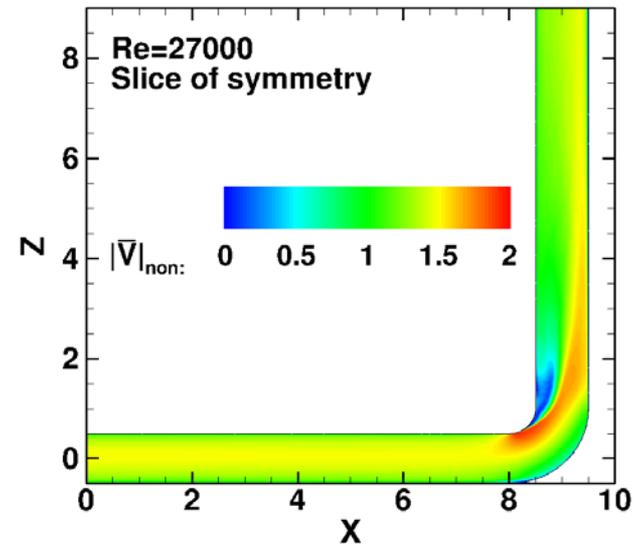
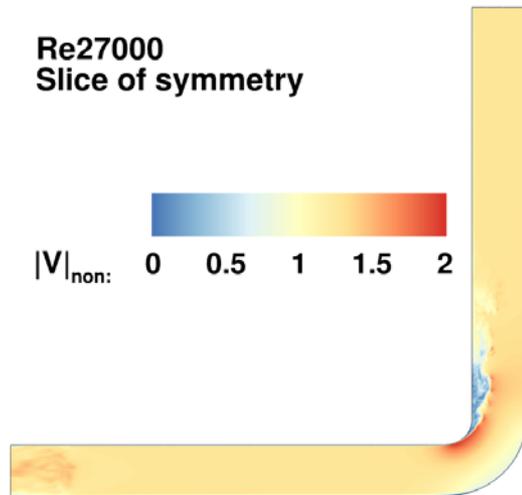


(b) Swirl switching (Vester et al. 2011)

- Steady Dean vortices are observed at downstream of a bend for laminar flows;
- Swirl switching is proved to exist for turbulent flows downstream of a bend.

Question: Could the swirl switching be one of the causes of the erosion?

Flow field visualization

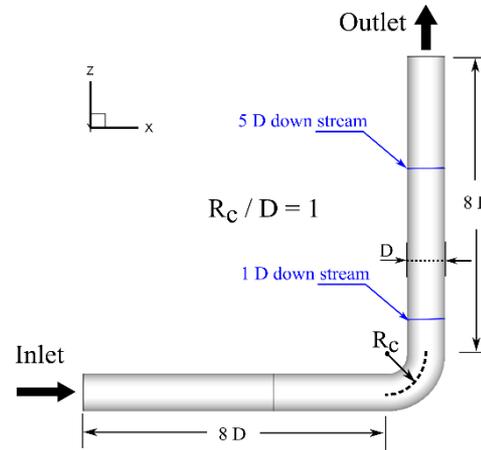
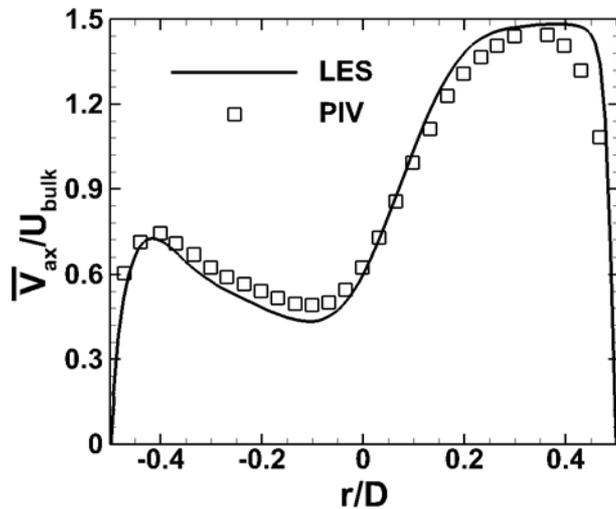


- Non-dimensional velocity magnitude at the center slice of the pipe;
- The pre-recorded inflow data provide a fully developed turbulent flow;
- Mean velocity magnitude becomes higher at the inner wall at 30 degree angle;
- At 90 degree, the maximum velocity shifts towards the outer wall.

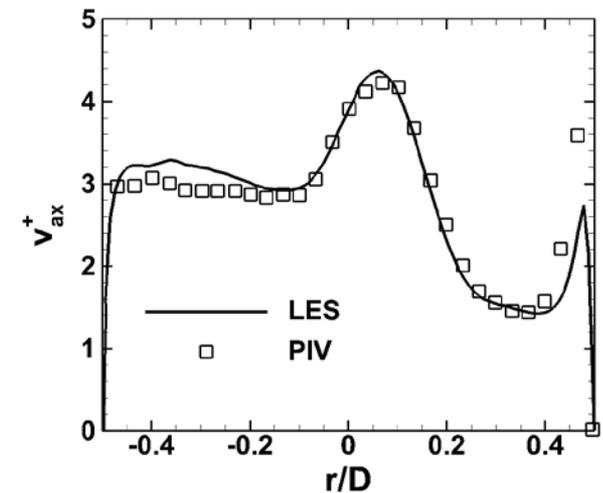
Validation

Mean and RMS velocity profiles after the bend (Re=5000)

(a) Mean velocity profile at 1D downstream of bend



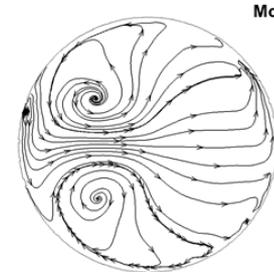
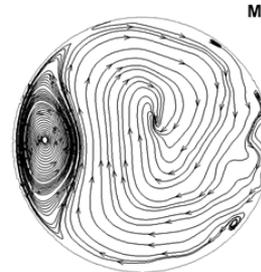
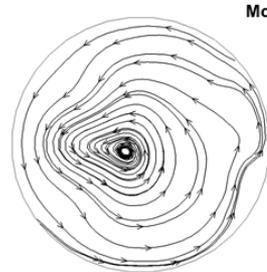
(b) RMS velocity profile at 1D downstream of bend



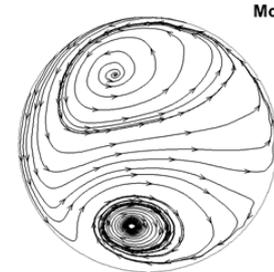
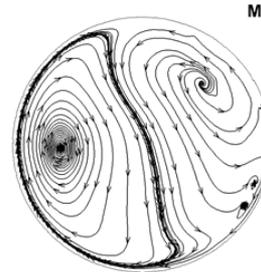
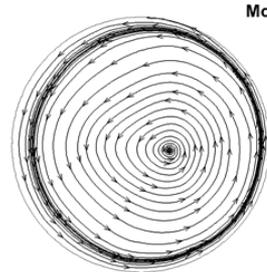
(PIV study: Vester et al. 2016)

Proper Orthogonal Decomposition (POD) modes

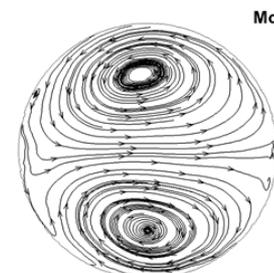
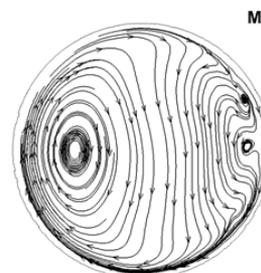
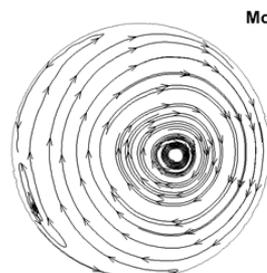
1D downstream



3D downstream



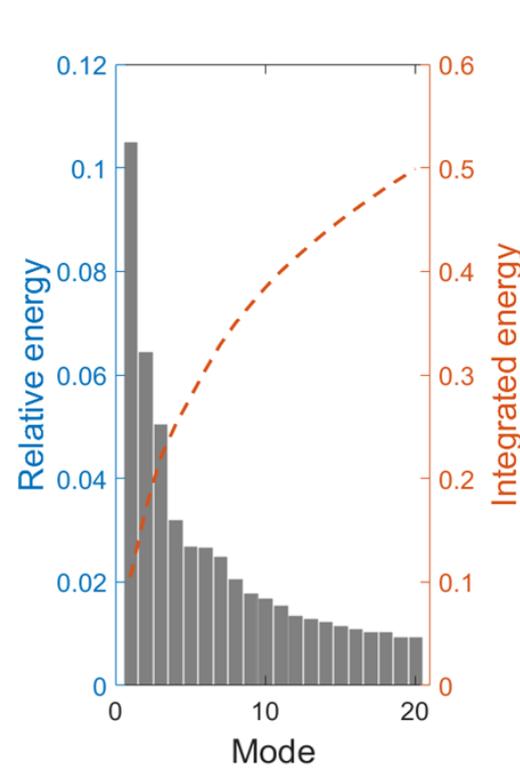
5D downstream



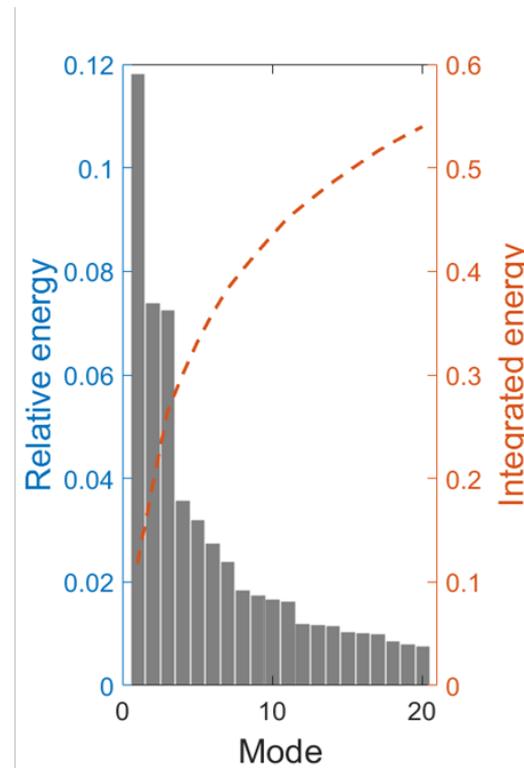
Swirling switching phenomenon was observed downstream of the bend for $Re=27,000$. Similar phenomenon is expected for higher Re cases.

Energy level for the POD modes

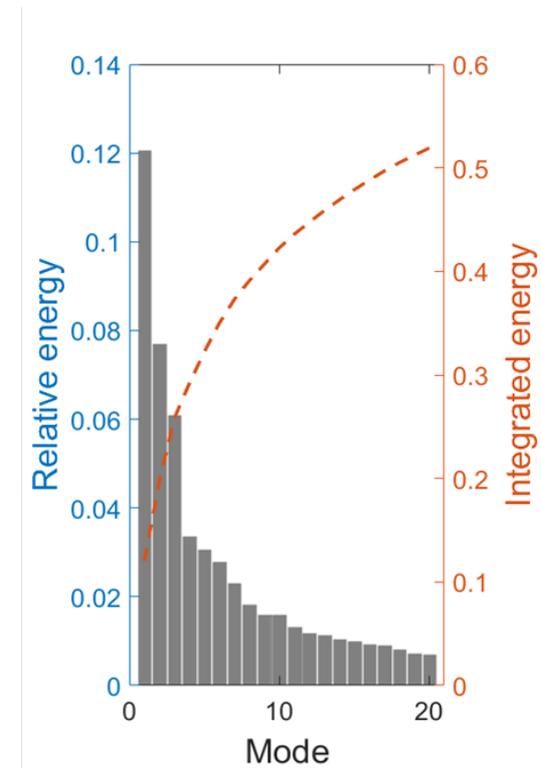
($Re=27000$)



1D downstream



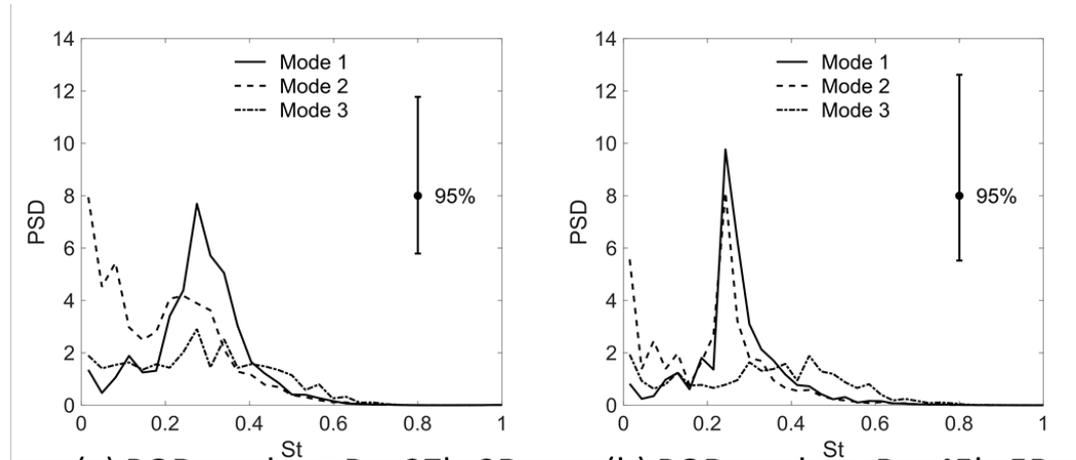
3D downstream



5D downstream

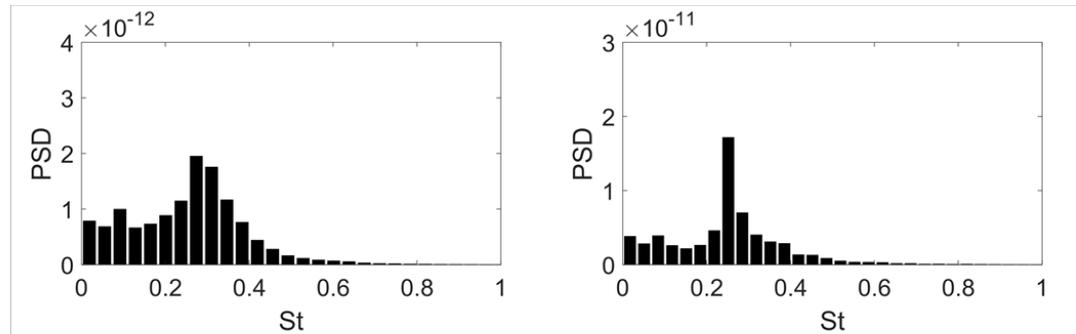
The first three modes are the most energetic modes.

Power Spectra Density (PSD) for the POD modes and shear forces



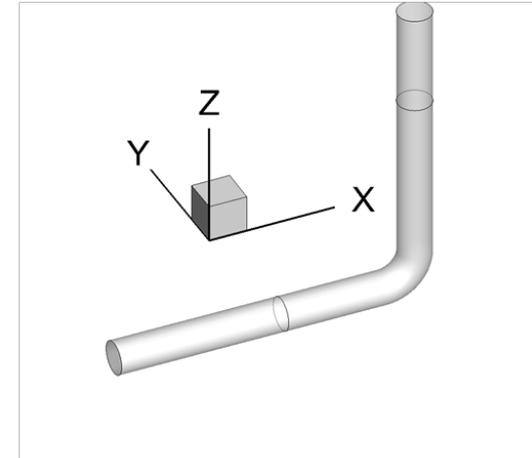
(a) POD mode at $Re=27k$, 3D

(b) POD mode at $Re=45k$, 5D



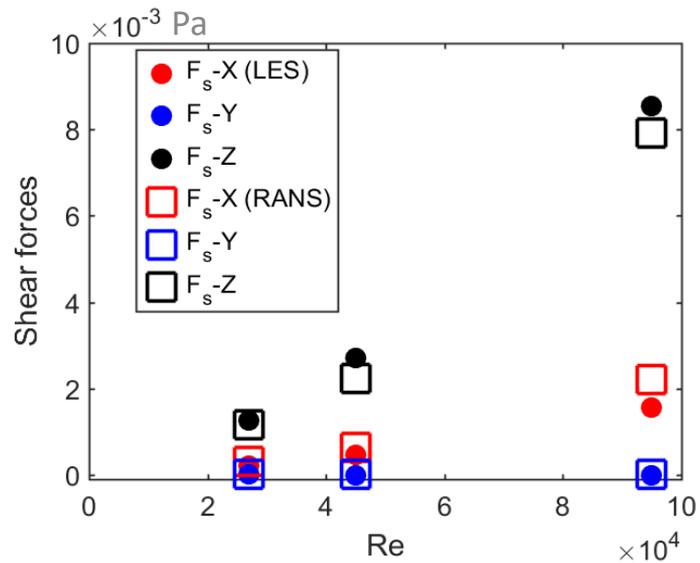
(c) Shear force in Z direction for $Re=27k$

(d) Shear force in Z direction for $Re=45k$

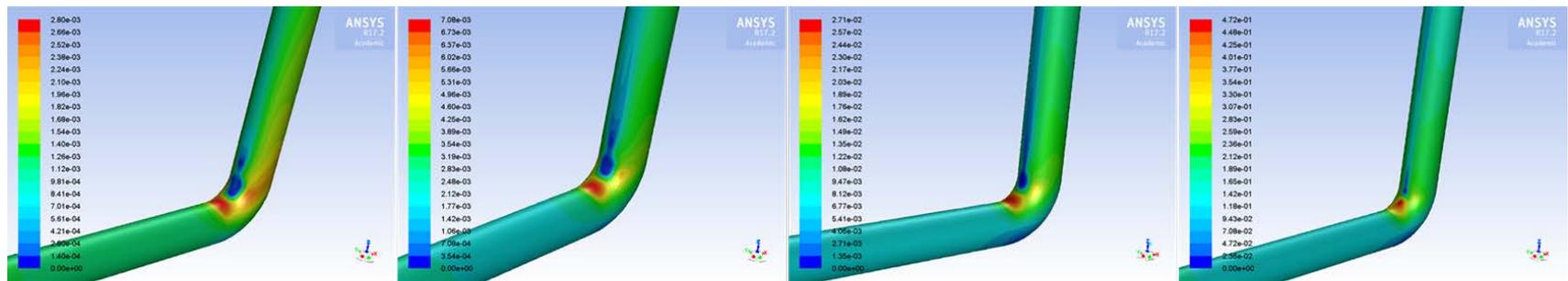


The frequency of the swirl switching matches with that of the total shear force in Z direction on the wall.

sCO₂ Flow in a Pipe Bend



Using CFD simulations, we showed that the oscillation of the secondary flow patterns directly causes the oscillation of the shear forces on component walls. This could result in erosion through spallation of oxide scale creating solid particles entrained in the sCO₂ flow which in turn causing erosion by particle impact.



Re=27000

Re=45000

Re=95000

Re=500000

The shear force at Re=15x10⁶ is likely to be responsible for the breakdown of oxide scale on the inner surface of a pipe

Observations of sCO_2 turbine degradation

Root cause of damage:

- Impact by solid particles?
- Fluctuating shear forces?
- Phase change?

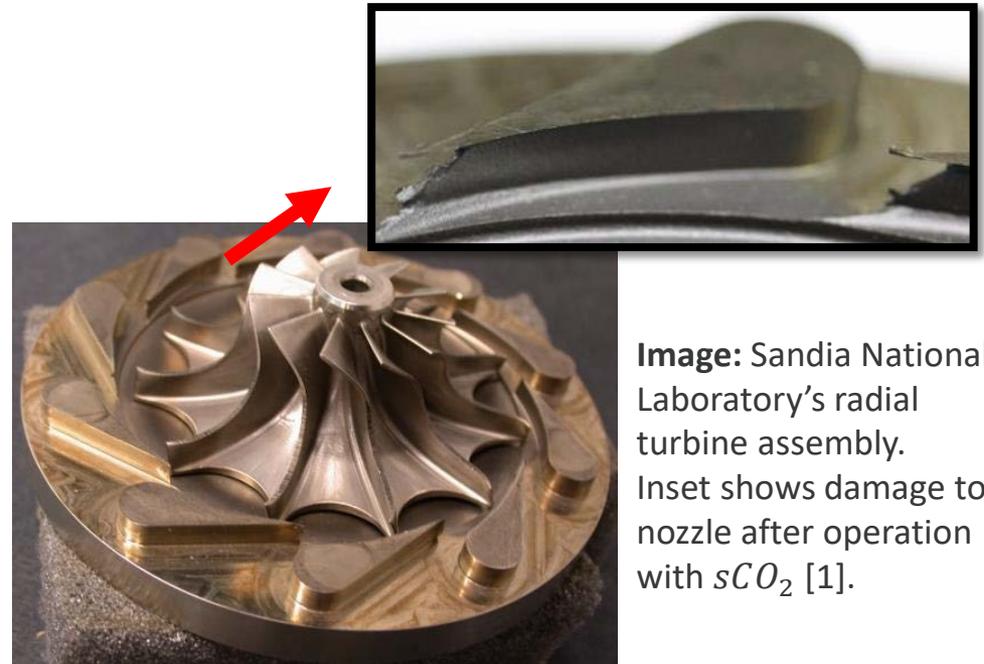
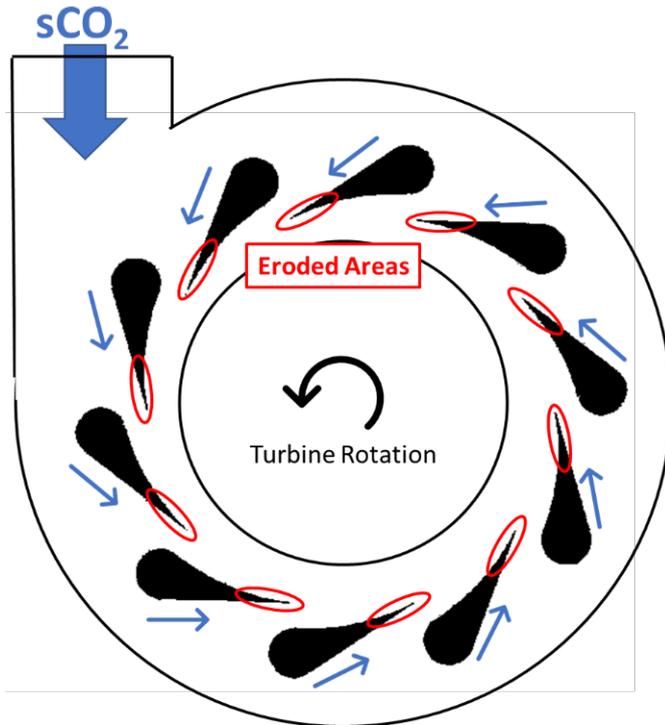
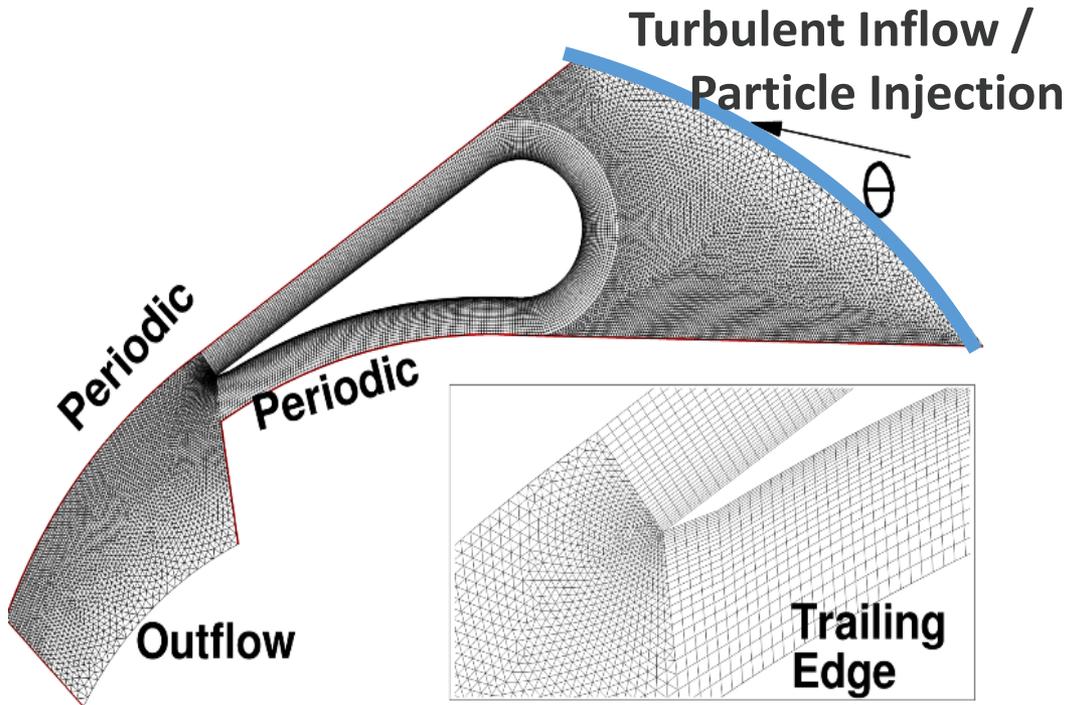


Image: Sandia National Laboratory's radial turbine assembly. Inset shows damage to nozzle after operation with sCO_2 [1].

Simulation Setup



2D cross section of single nozzle passage showing periodic approximation and unstructured, body fitted grid.

Geometry

- Single passage of 3D SNL nozzle
- Flow through turbine wheel and casing not considered

Unstructured Mesh

- Structured (hex) O-grid topology near nozzle surface
- Unstructured (prism) cells upstream/downstream
- Wall normal grid spacing, $\Delta_n^+ = 1$. Span-wise/chord-wise spacing of $\Delta_c^+ = \Delta_s^+ = 6$.

Turbulent inflow condition

- Mean inflow angle, $\theta = 20^\circ$
- Synthetic eddy method¹ for turbulent inflow

Solid particles

- Random injection at inflow plane
- Continuous injection to maintain $\langle\langle \varepsilon_s \rangle\rangle = \frac{v_p}{v_{domain}} = 10^{-4}$

Simulation conditions

Video: Simulated particle trajectories (magenta) and vortex swirling strength



Assumed Operating Conditions (125kWe SNL test facility)

- Nozzle chord length $L \approx 2.5\text{cm}$, height $h \approx 0.4\text{cm}$
- Flow rates in the neighborhood of $\dot{V} = 600\text{GPM}$
 - Velocity at nozzle tip, $u_{bulk} = 45\text{m/s}$
- Turbine inlet conditions : $T = 550^\circ\text{C}$, $P = 29.11\text{MPa}$
 - $\rho = 177 \frac{\text{kg}}{\text{m}^3}$, $\mu = 39 \times 10^{-6}\text{Pa} \cdot \text{s}$
- Reynolds number: $Re_c = \frac{\rho \cdot u_{bulk} \cdot L}{\mu} \approx 5 \times 10^6$

Simulation conditions

- LES of operational Re_c expensive without wall modeling
- We are developing simulation framework at $Re_c = 11,000$

Solid particles

- Source: spallation of porous oxide scales
 - $\rho_p = 2500 \text{kg/m}^3$, $d_p = 30\mu\text{m}$
- Stokes Number (measure of particle inertia/relative velocity)

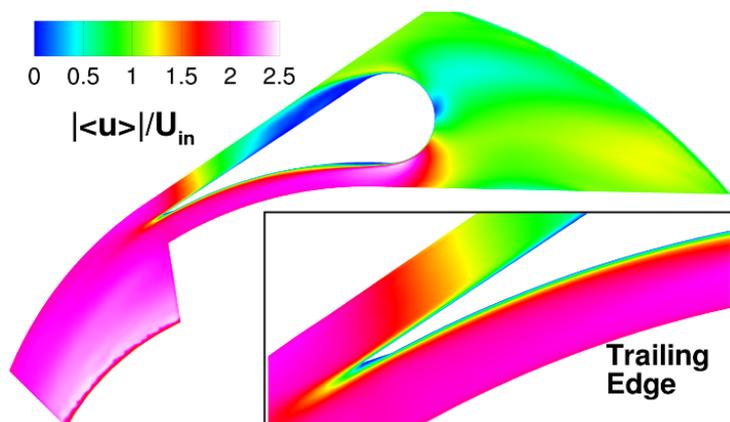
$$St_p = \frac{\tau_p}{\tau_k} = 1.5$$

Table: Simulation parameters

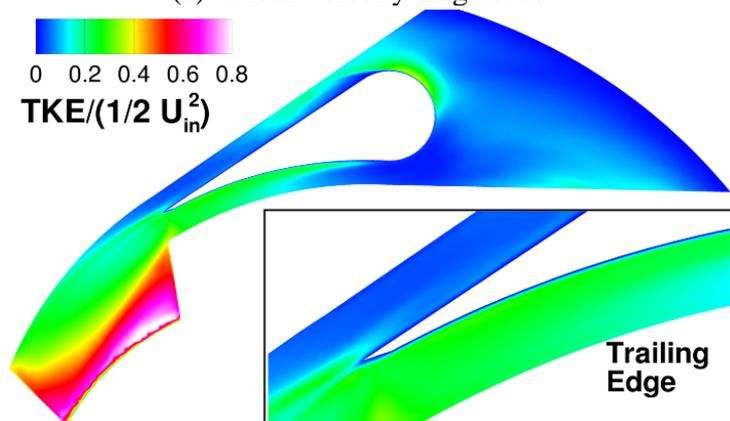
	sCO ₂		Particles
ρ	$177 \text{kg} \cdot \text{m}^{-3}$	ρ_p	$2500 \text{kg} \cdot \text{m}^{-3}$
μ	$39 \times 10^{-6} \text{Pa} \cdot \text{s}$	d_p	$30\mu\text{m}$
θ	20°	St_p	1.5
U_{in}	$0.1 \text{m} \cdot \text{s}^{-1}$	$\bar{\varepsilon}_s$	10^{-4}
u_{bulk}	$0.22 \text{m} \cdot \text{s}^{-1}$	dt_p	$2 \times 10^{-6}\text{s}$
Re_c	11,000		
dt_f	$2 \times 10^{-5}\text{s}$		

Results: Mean flow and particle concentration

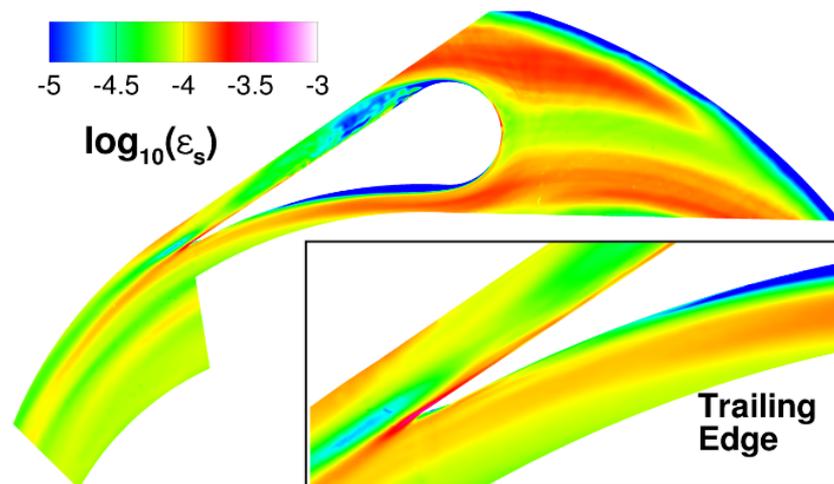
All fields time averaged over $\frac{tU_{in}}{L} = 10$ non-dimensional time units



(a) Mean velocity magnitude



(b) Turbulent Kinetic Energy



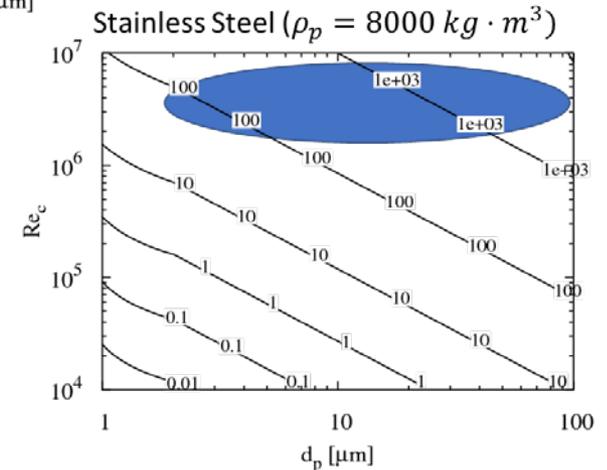
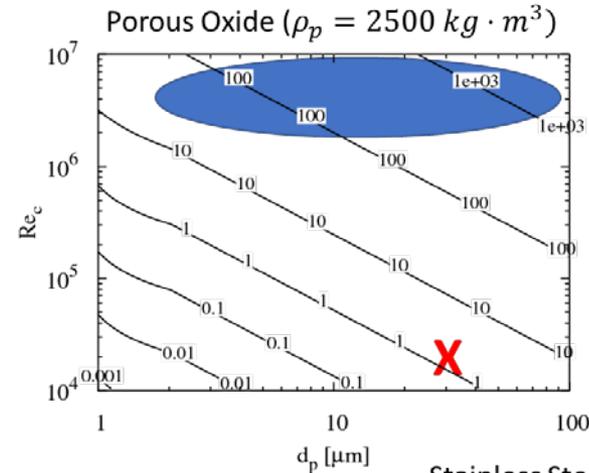
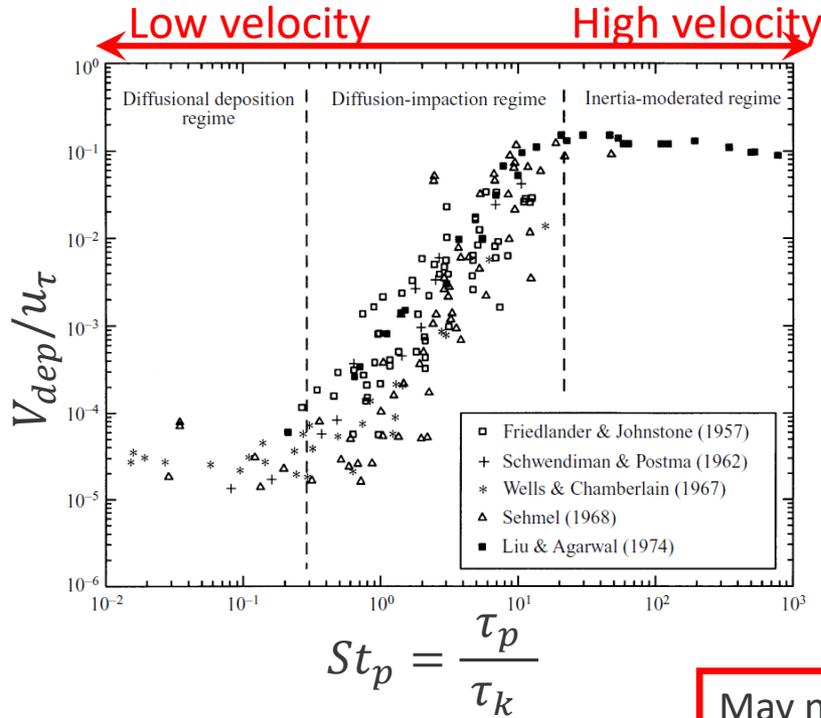
(c) Particle solid fraction (log scale)

- Flow acceleration, increasing TKE along pressure side of nozzle passage
- Particles tend to travel near surface of trailing edge on both pressure and suction sides

Implications for operational Reynolds numbers

Particle impact velocity depends primarily on St_p ¹

St_p scales with d_p and Re_c for this system



May need to filter very small particles from flow loop to avoid high velocity impacts!

Ongoing work

- **Simulate operational Reynolds numbers ($>10^6$)**

Employ combination of RANS/LES (ie, Fluent) if LES proves computationally expensive

- **Estimate erosion rates from particle impact data**

Semi-empirical models available to relate rate of material erosion to kinetic energy of particle impact ($|\mathbf{u}_p|^2$), and impact angle, α

$$E = k|\mathbf{u}_p|^2 f(\alpha)$$

- **Simulate full 360 degree nozzle passage**

