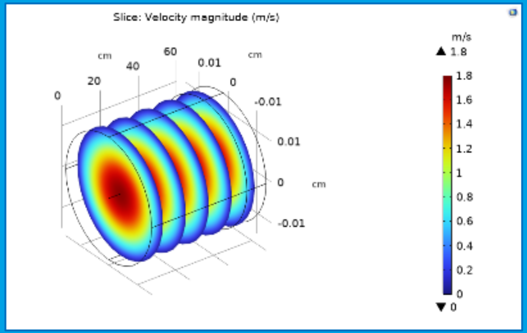
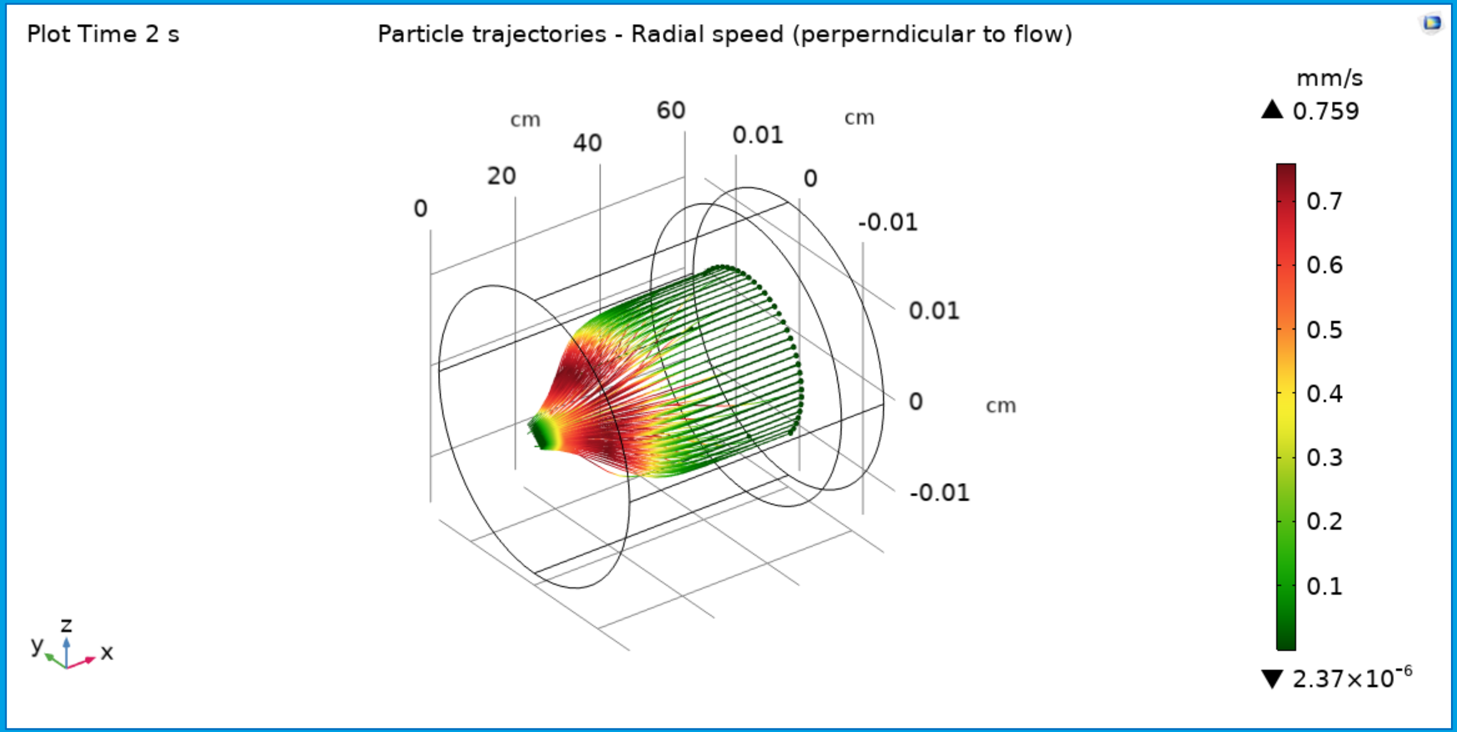
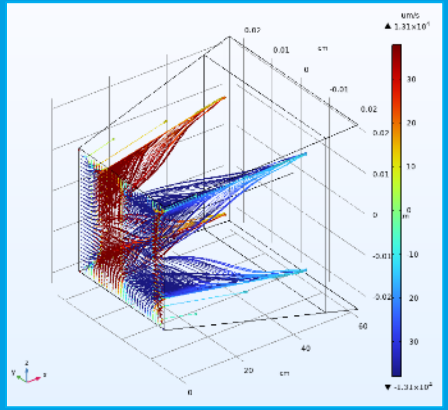






Guido Spinola Durante
Expert R&D Engineer

26.10.2023

MULTIPHYSICS INERTIAL PARTICLE FOCUSING (IFP) MODEL VALIDATED FOR 3D MICRO-FLUIDIC GEOMETRIES

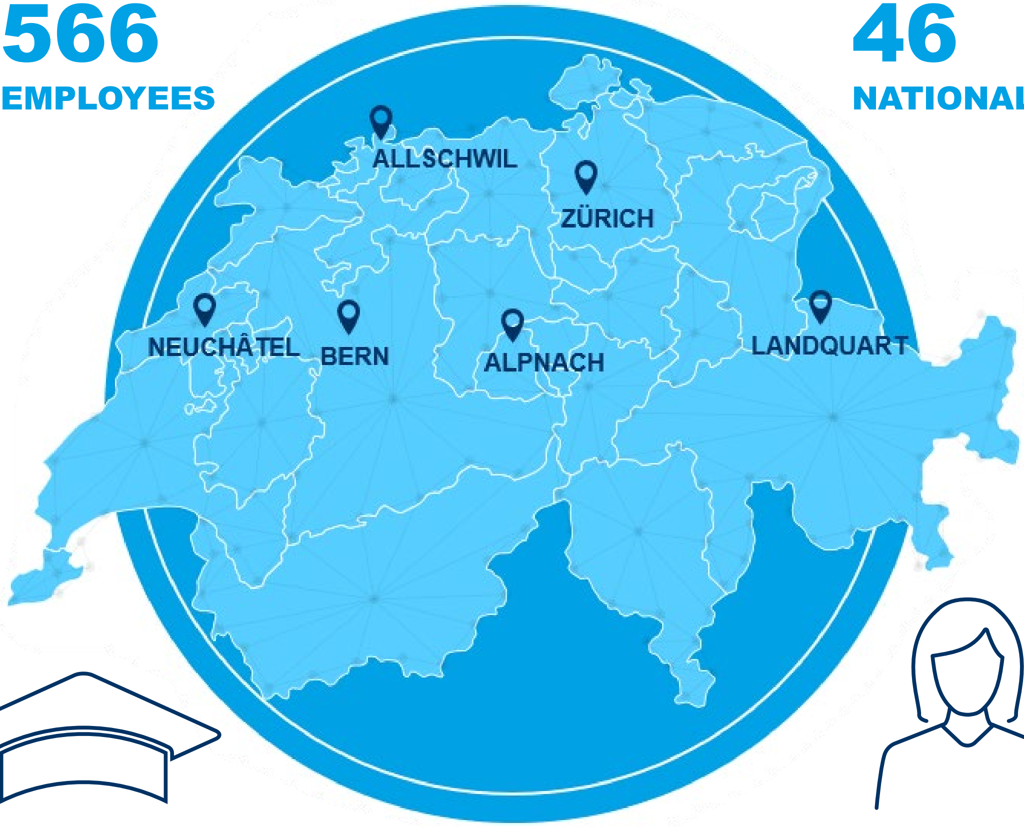
CSEM AT A GLANCE

We are a public-private, non-profit, Swiss technology innovation center.

We enable competitiveness through innovation by developing and transferring world-class technologies to industry.

566 EMPLOYEES

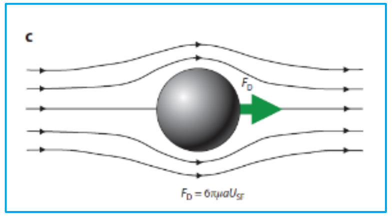
46 NATIONALITIES



35% PHD

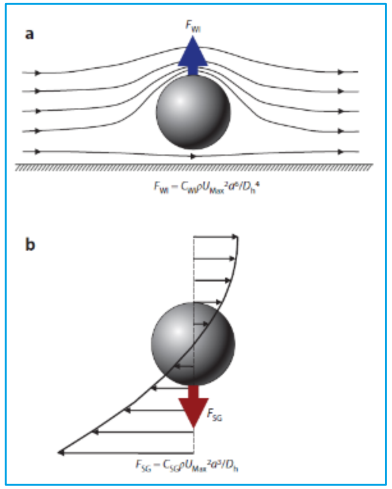
28% WOMEN

INERTIAL PARTICLE FOCUSING (IFP) - PROBLEM STATEMENT



Stokes Drag (1851)

- Drag force (F_D) of the fluid flow is acting on particles
- Lift force (F_L) is pushing particles away from the walls and gently away from the position of maximum speed in the cross-section



- Secondary Dean flow with vortex formation in the cross-section can scatter particles around and facilitate mixing / migration of particles from inner to outer radius in a curve. It is characterized by Dean Number De=Re*sqrt(D/(2*Rc))
  This effect is included in the drag force (F_D) of the fluid flow on particles
- All the above effects combined will impact particle focusing

When does IFP happen?

- Criteria 1: (r_p/Dh) > ~0.07
  Note: (r_p /Dh) < 0.2-0.5 avoid channel obstruction
- Criteria 2:De < ~30
- Onset of IFP does not give any hint on timing, length, complexity of the focusing patter.
  -> FEM simulation is needed to support design

Why is it important ? Literature available (2019)

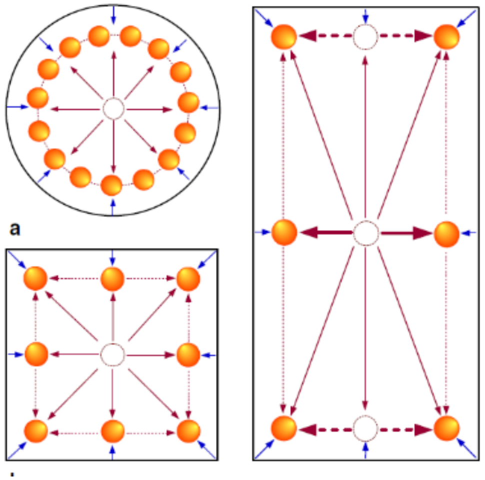
- https://www.nature.com/articles/s41598-019-52983-z
  - **micro-cell sorting / Lab-on-chip / other**
  - **complex behavior Re up to 100**
  - **zig-zagging fluidic channels**

COMSOL MODEL AVAILABLE AND ITS LIMITATIONS

- The validated inertial particle focusing Comsol model is only in 2D
- The model is based on **lift-force** boundary condition implemented only for parallel walls in 2D/3D
- Gentle change in the cross-section along the fluid channel path cannot be modeled directly with implemented Comsol feature.
- **Developed here: lift force based on wall-distance physics for constant/slowly-variable channel width – (but missing high-order fluid speed correctionin lift-off forces in curves)**

Segré-Silberberg effect of inertia-induced lateral

Particle focusing patterns



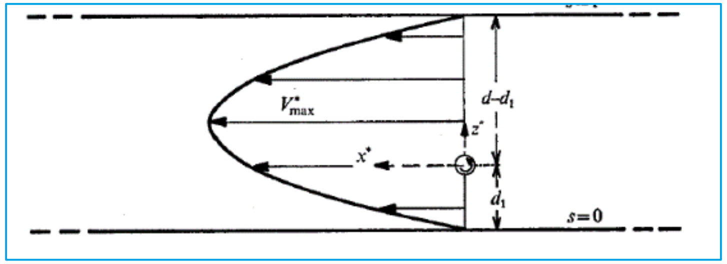
Comsol benchmark model:

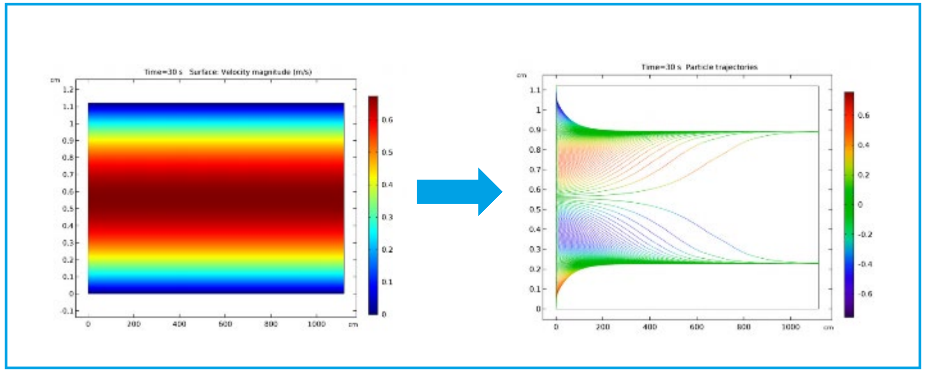
$$F_L = \rho \frac{r_p^4}{D^2} \beta(\beta G_1(s) + \gamma G_2(s))\mathbf{n}$$

$$\beta = |D(\mathbf{n} \cdot \nabla)\mathbf{u}_p|$$

$$\gamma = \left|\frac{D^2}{2}(\mathbf{n} \cdot \nabla)^2 \mathbf{u}_p\right|$$

$$\mathbf{u}_p = (\mathbf{I} - (\mathbf{n} \otimes \mathbf{n}))\mathbf{u}$$



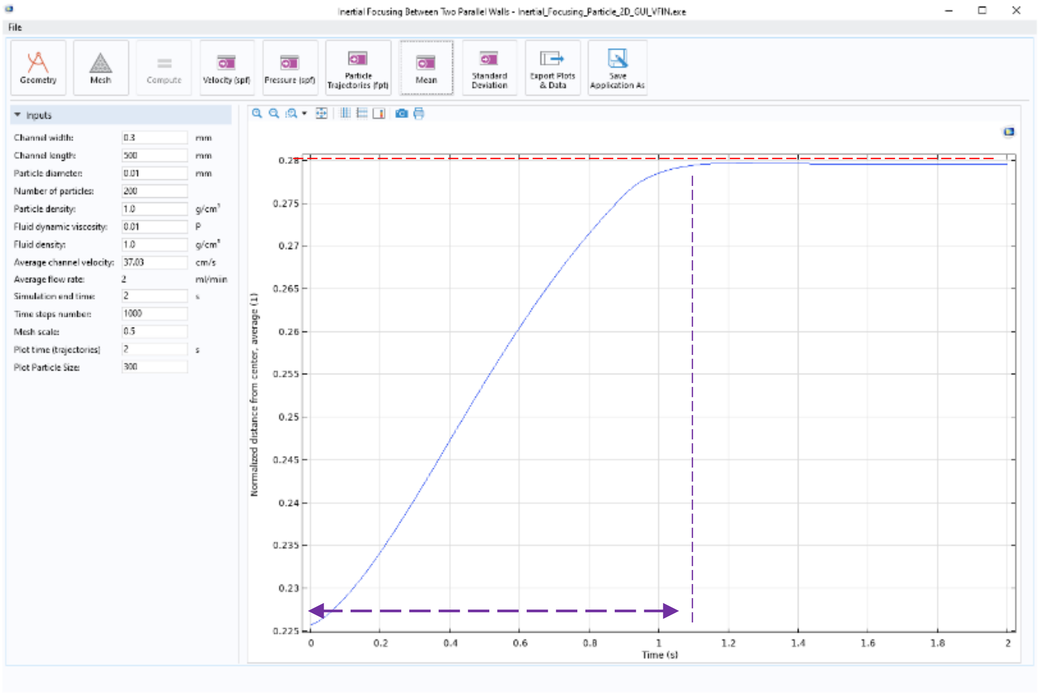


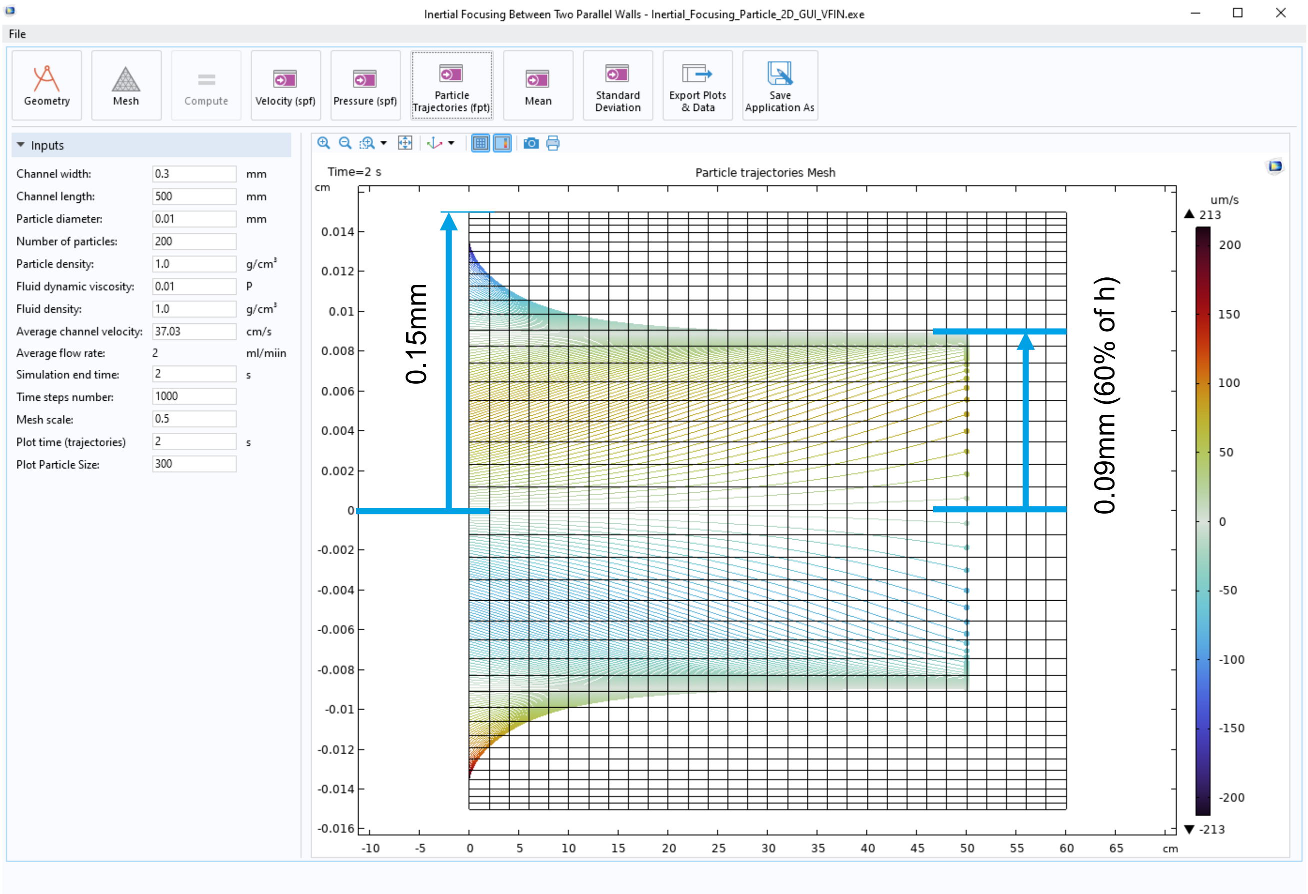
Comsol tutorial model

GUI MODEL DEVELOPMENT AND VALIDATION STRATEGY

- Reproduce results of 2D GUI model with a 3D cylinder model / 3D trapezoidal pipe with increasing cross-section

- Check 1D/2D **particle normalized average distance from axis** in the output cross-section





COMSOL 2D model -> turned into GUI

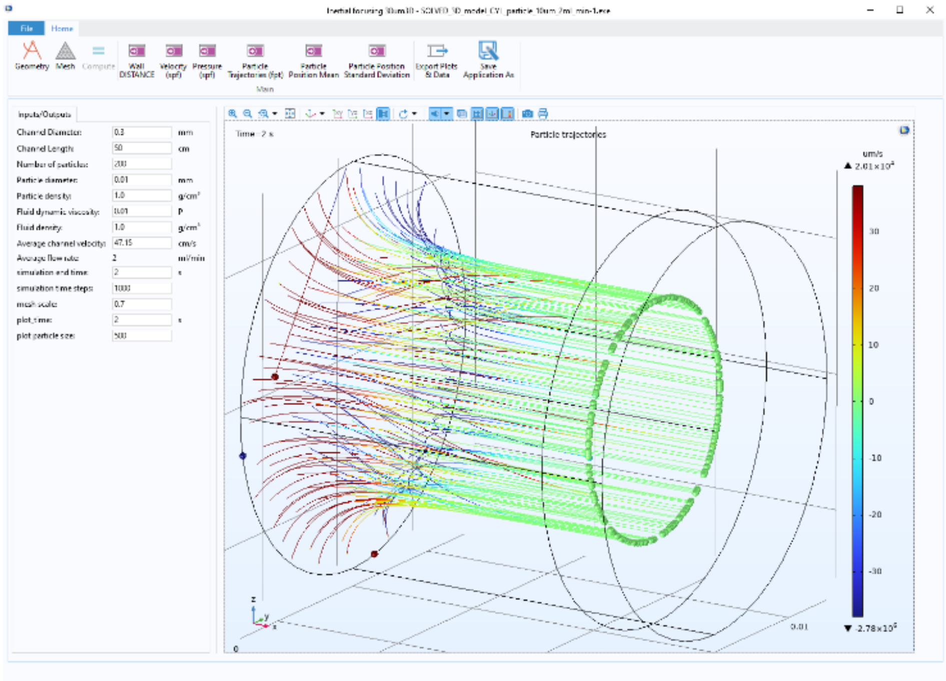
3D GUI MODELS WITH CONSTANT/VARIABLE CROSS-SECTION

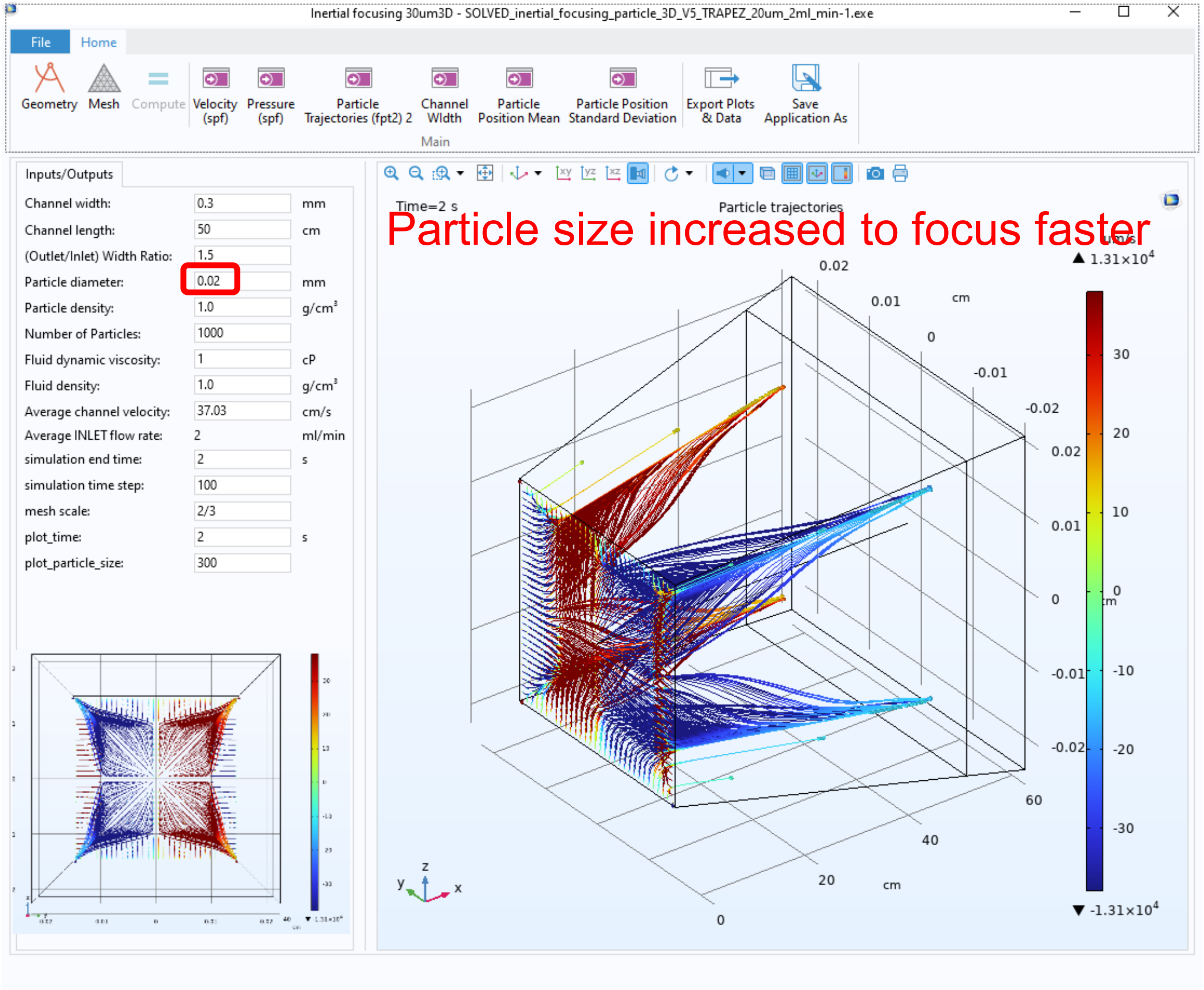
Added lift force feature coupled to wall interface physics: constant channel width

- 3D cylinder model shows the typical expected ring focusing behavior

Added lift force feature coupled to wall interface physics: variable channel width

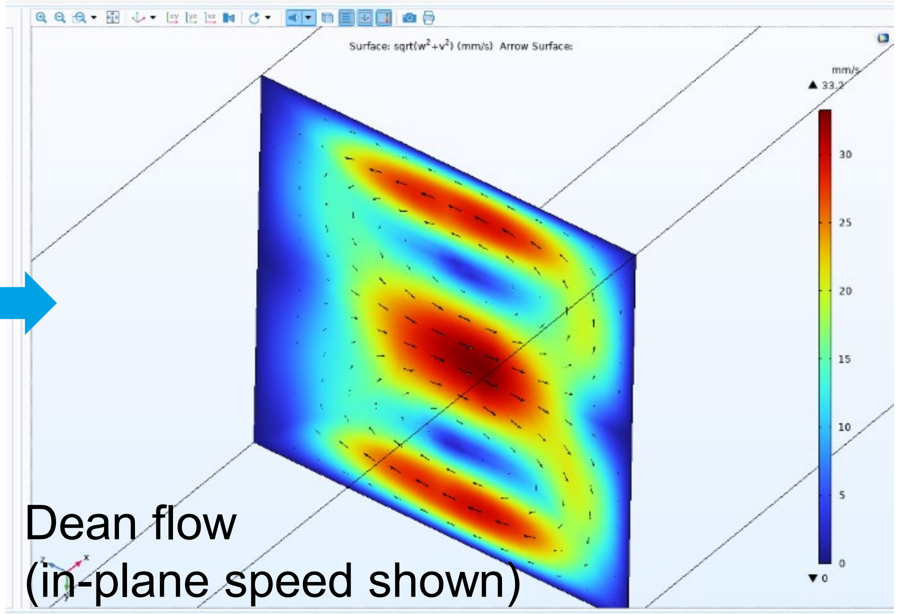
- 3D trapezoidal pipe with increasing cross-section shows reduced focusing with widening channel



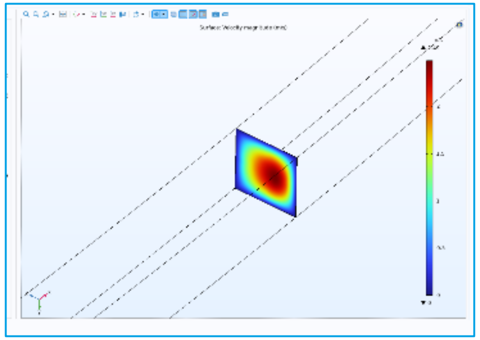


3D SECONDARY (DEAN) FLOW IN CURVED MICRO-CHANNELS

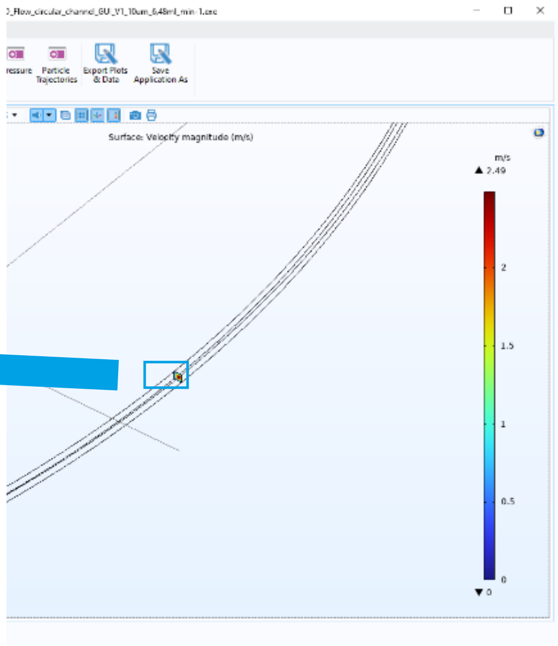
- Dean flow with two recirculating vortex in the cross-section
- Effect of Dean flow is that particle release in a point at the inlet tend to rotate and spread in-plane.
- **Higher order speed profile corrections to lift-forces in curves are not implemented yet**

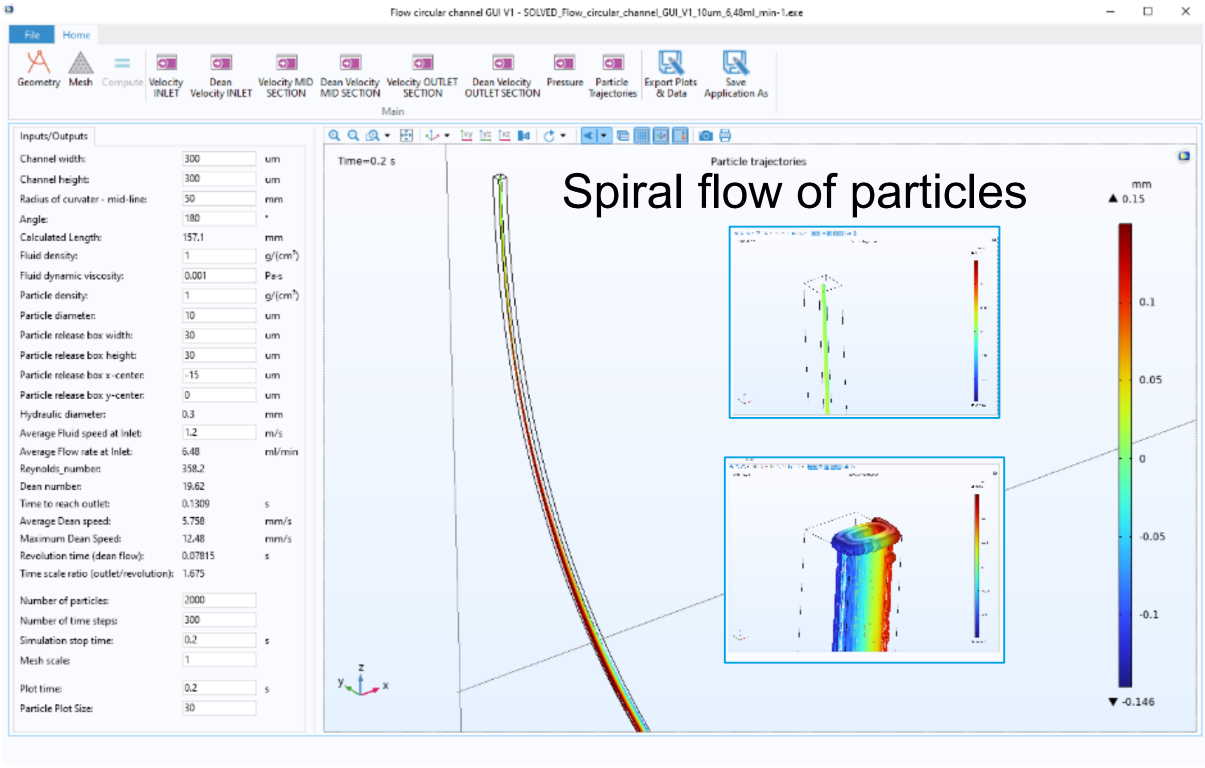


Dean flow
(in-plane speed shown)



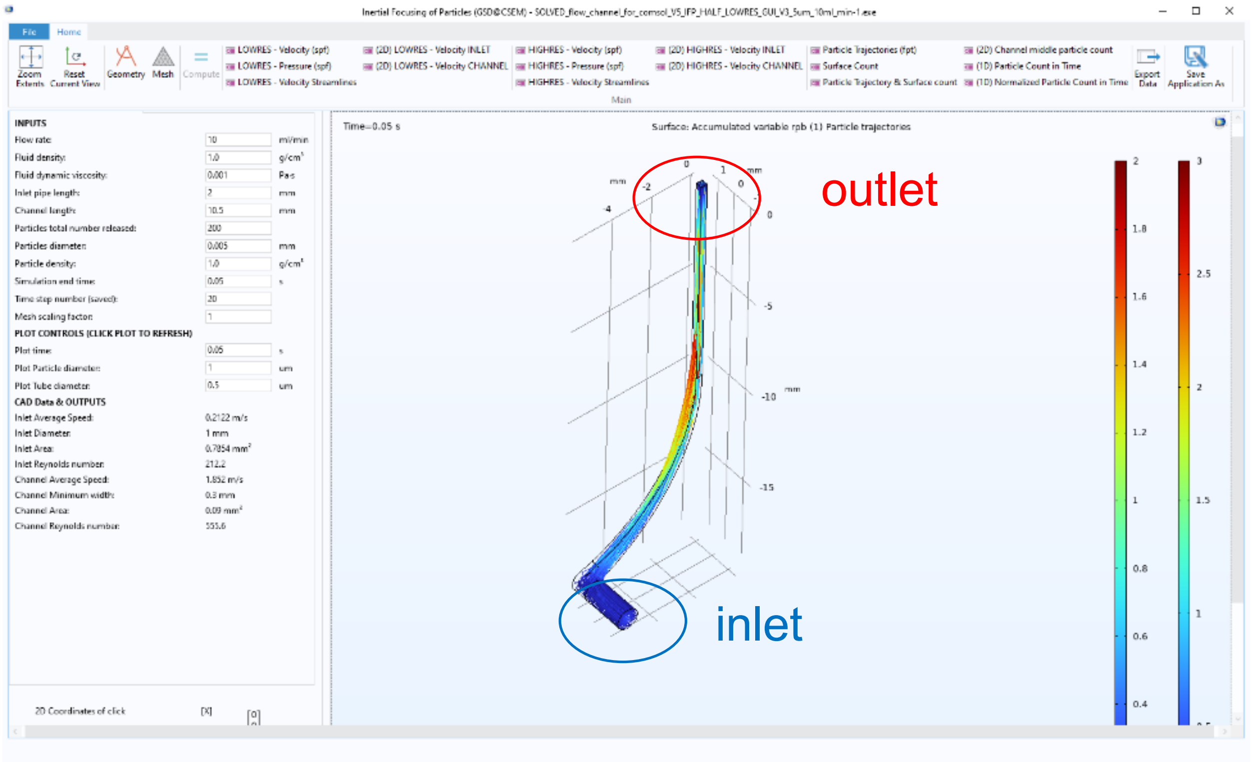
Non-purely symmetric flow (lift-force offset in curved channels)



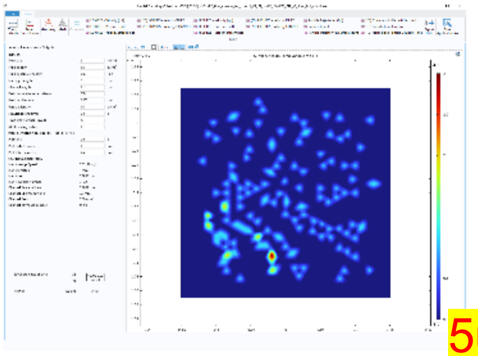


3D GUI MODEL BASED ON CAD MODEL

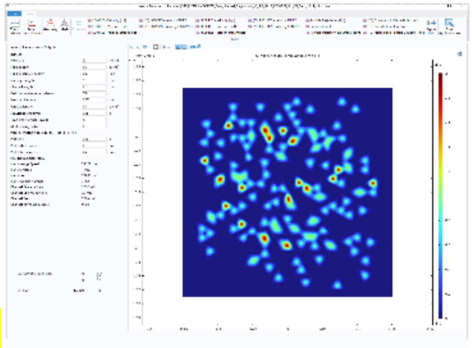
- Full 3D model with <u>parametrized inlet length</u> <u>(</u>round pipe) <u>and</u> straight channel <u>outlet length</u>
- Model is fully parametrized can be used for evaluating different particle size/density, fluid flow conditions, simulation times
- Data can be picked and visualized directly in the graphic windows
- All plots and data and the solved model itself can be saved.
- Model runs in ~2h on fast PC with 64GB ram



1ml/min

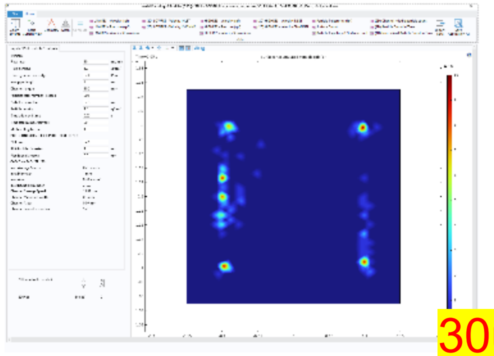


10ml/min

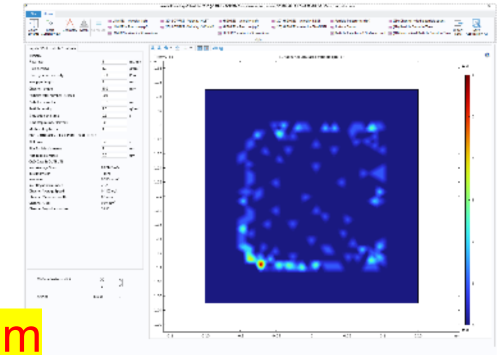


5um

1ml/min



10ml/min

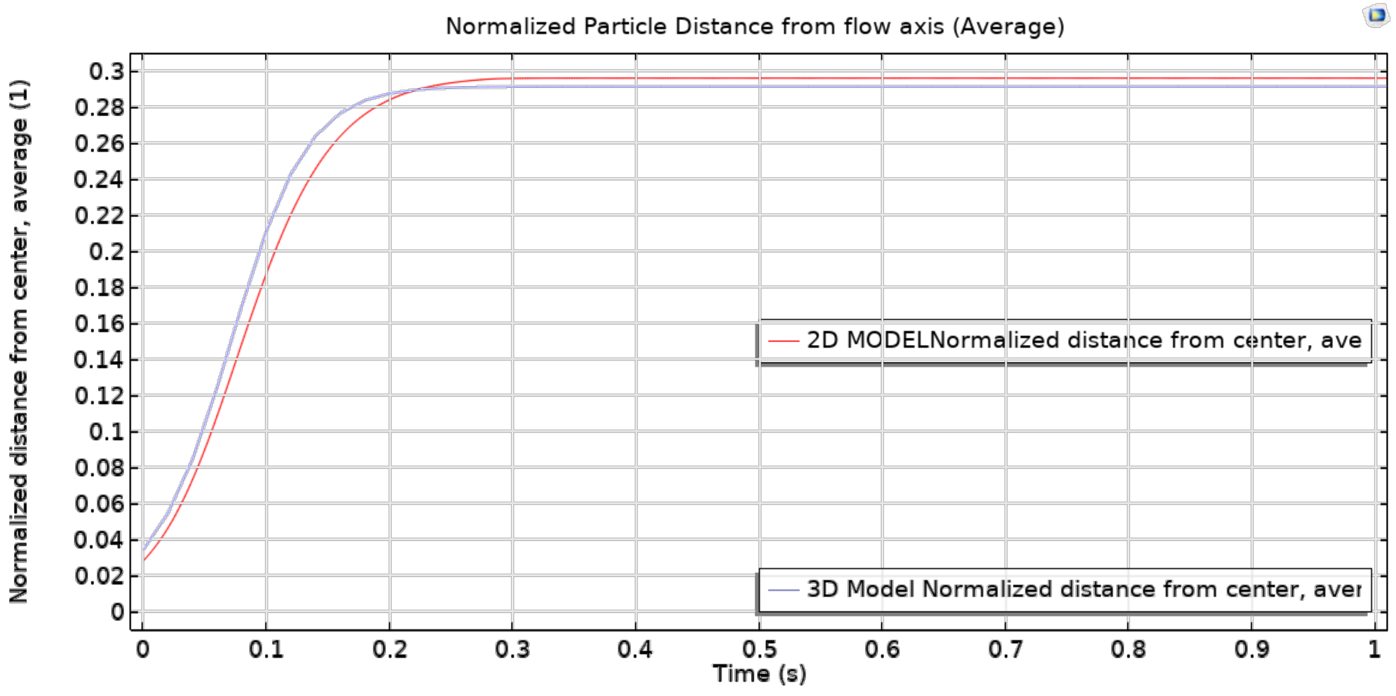


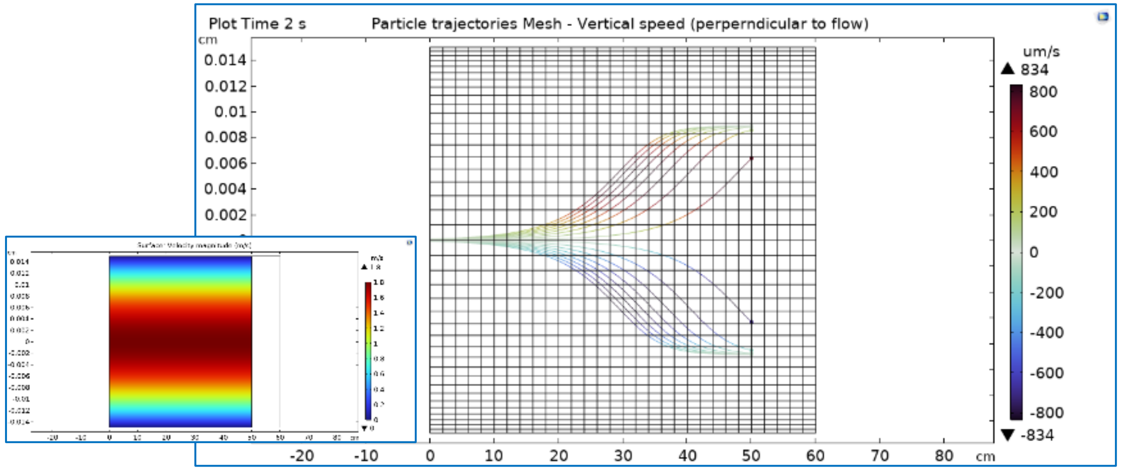
30um

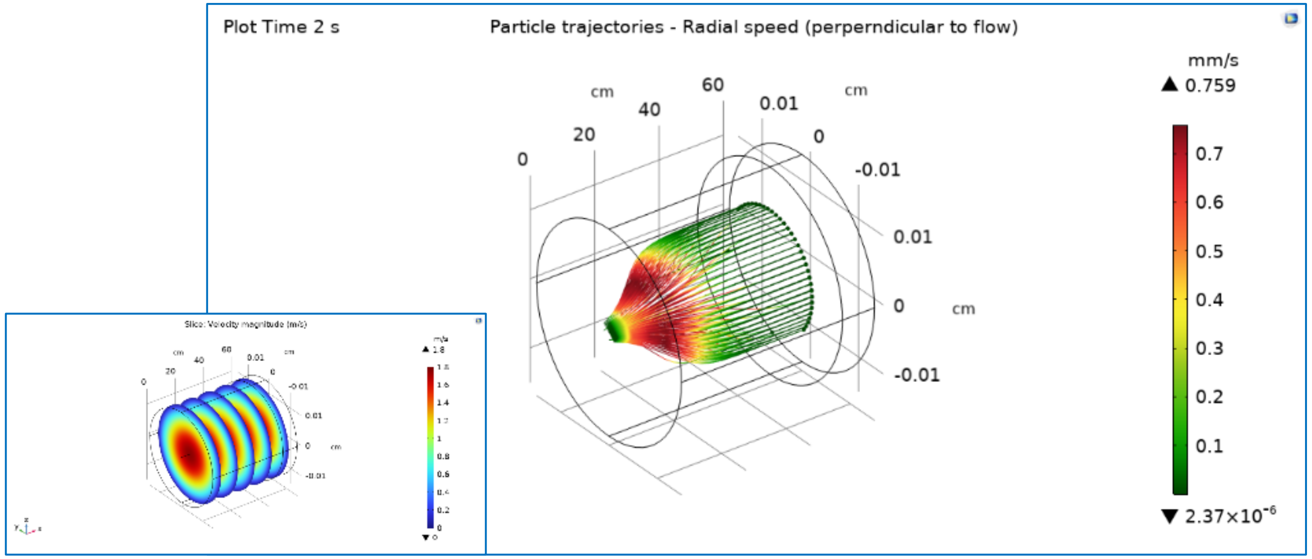
IFP TIMING VALIDATION

Comparison 2D/3D models:

- same maximum fluid speed
  -> keep same speed gradient
  on channel cross-section
- Initial release of particle from axis
  -> avoid particle non-uniform contribution to
  average distance to axis
- same axis-wall distance (equivalent radius)



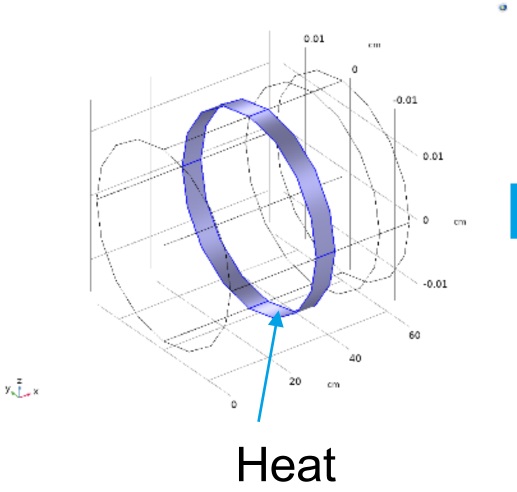


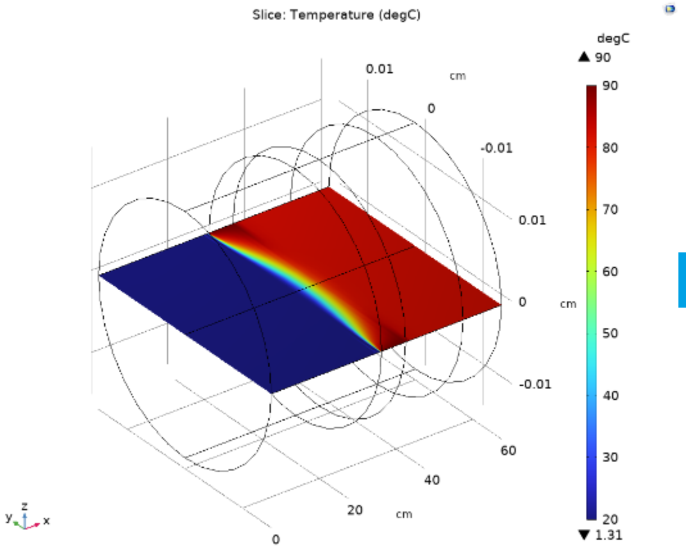


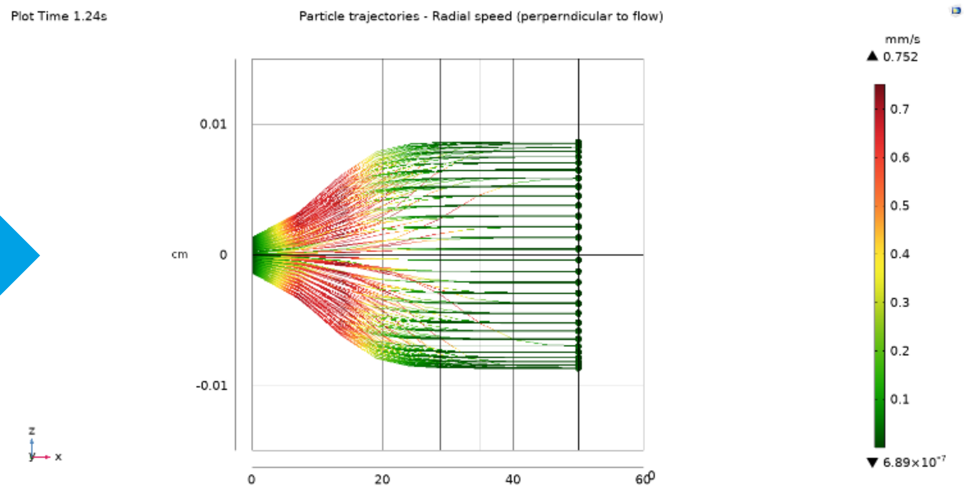
IFP MULTIPHYSICS COUPLING WITH THERMAL MODEL

- Laminar, Thermal, Particle phyiscs coupled
- Thermal gradient or fluid/particle properties change with temperature can offset particle focusing
- The relevant effect is to change the focusing position at the outlet

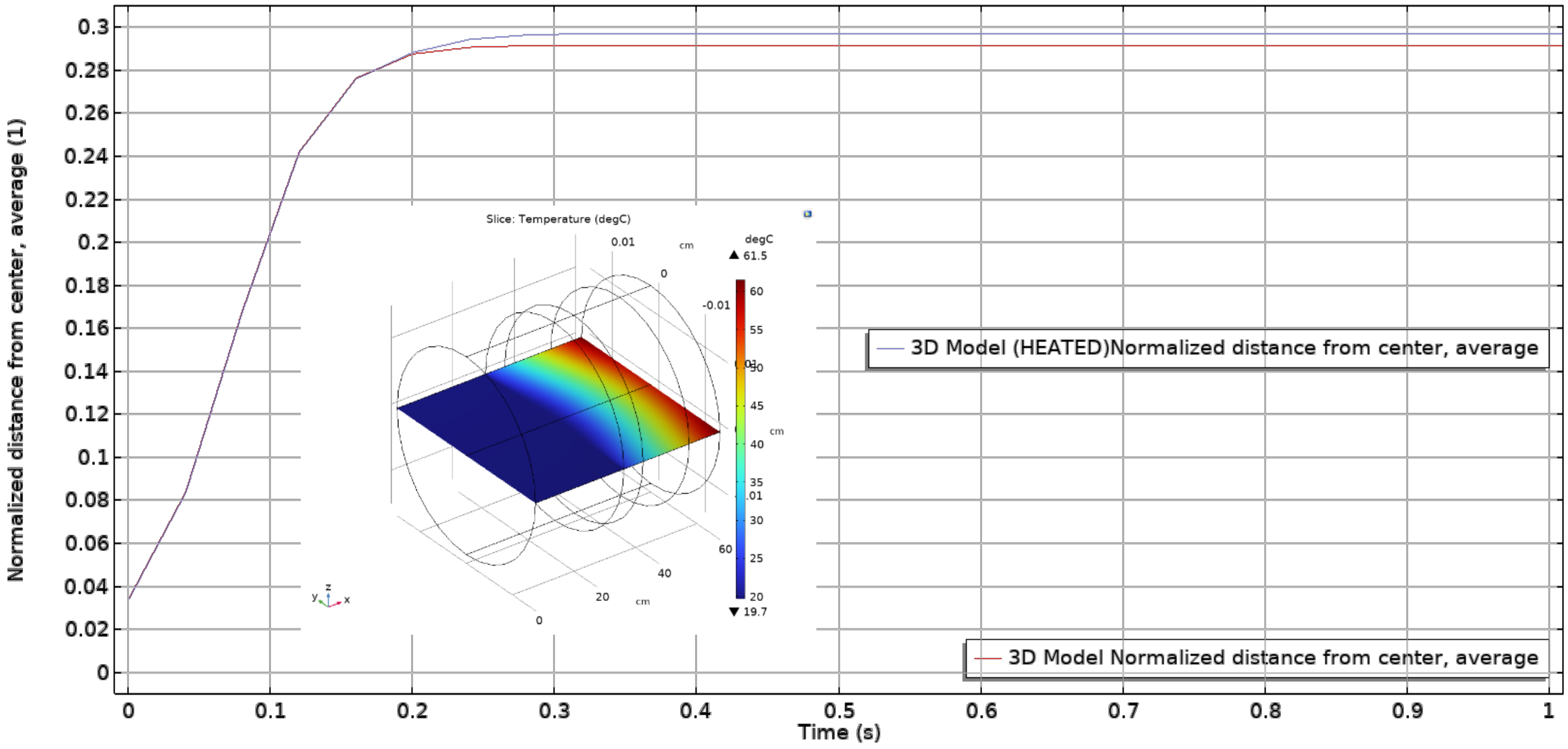
➡ relevant for IFP design – 19 minutes simulation time (0.3mm OD, L=60cm)







IFP MULTIPHYSICS COUPLING WITH THERMAL MODEL
HEATED/NON-HEATED RESULTS COMPARISONS



CONCLUSIONS & NEXT STEPS

Conclusions

- Comsol modeling strategy and ist validation was implemented for 3D cylindrical and 3D rectangular cross-section geometries with variable channel width, starting from Comsol 2D IFP benchmark model.
- The implemented approach can be used to model inertial particle focusing with any particle size/density and generic channel cross-section to support advanced micro-fluidics design apps.
- Multi-physics coupling with thermal model is possible and simulation time is fast ~19min. (no thermal pulses)

Next steps

- Validation of the thermal model coupled with IFP model.
- The approach can be further refined to add higher order correction in lift-force due to curves
  → solve IFP problem for generic **zig-zagging fluidic channels**
- The GUI can be automated to import any generic model from CAD
  → **requires dynamic definition of domains / inlet / outlet**

csem

FACING THE CHALLENGES OF OUR TIME