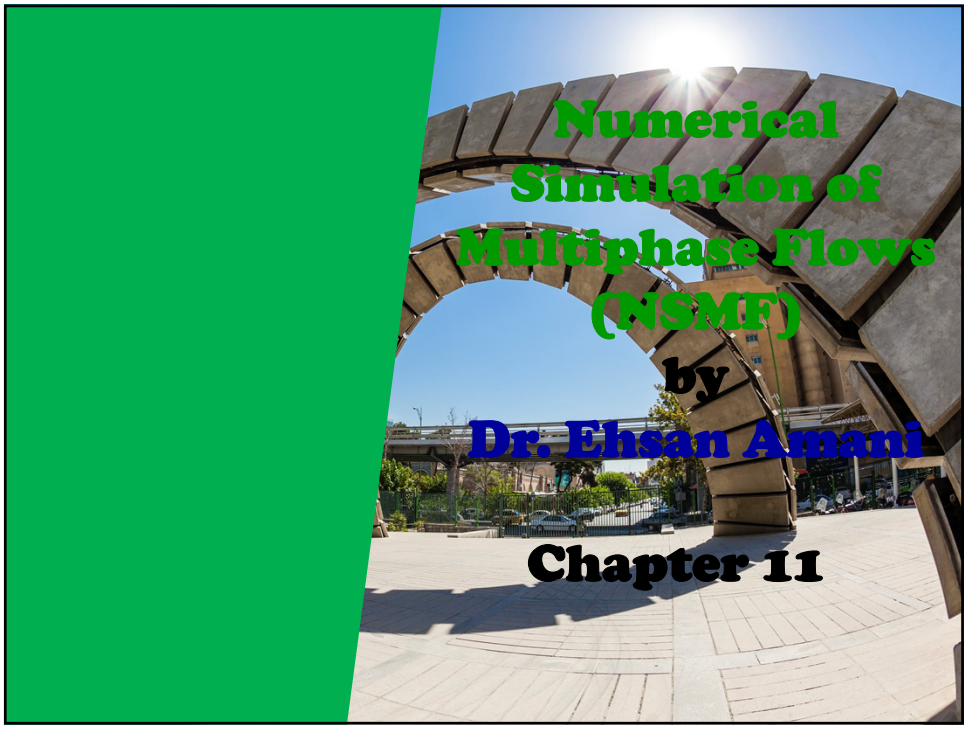

Initial condition – injection models

- Importance:
  accurate particle evolution calculation
  + inaccurate initial condition
  = ?!!!
- Goal:
  - Determining the state vector for each parcel

$$(\boldsymbol{x}_p, \boldsymbol{u}_p, d_p, \dots, \boldsymbol{u}_s, \dots, w_p)$$

- Injection model:
  - A part or the whole of the following flowchart

Injection modeling hierarchy

Simpler initial condition

Direct inputs

Injector specification

ΔP_{inj}, Geometry (d_{nozzle}, L), …

Injector models

Empirical correlations, stability analysis, …

Injection statistics

$\dot{m}_p$ or n_p or C_{Mp}
$f(d)$ or $(\bar{d}, \sigma, \dots)$
f_{du} or …
…

Computational parameters

Δt_{inj}, N_{inj}

Stochastic processes

$x_p, u_p, d_p, \dots, w_p$

inlet

Injection algorithm

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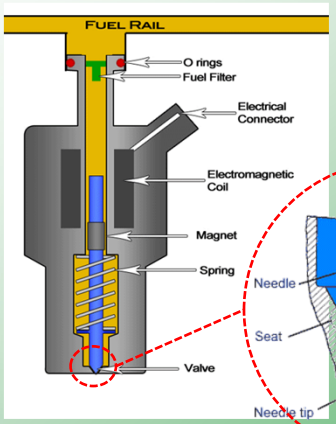
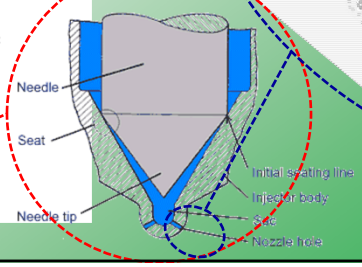
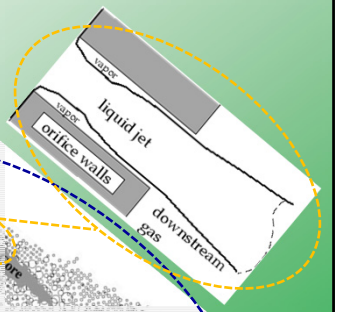
By E. Amani

Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
  - (Plain-)orifice atomizers







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Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
  - (Plain-)orifice atomizers

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Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
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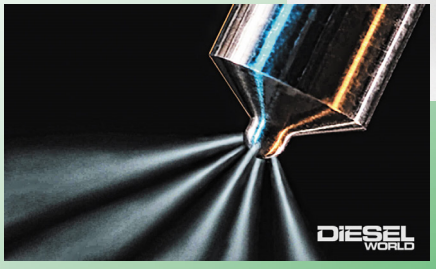

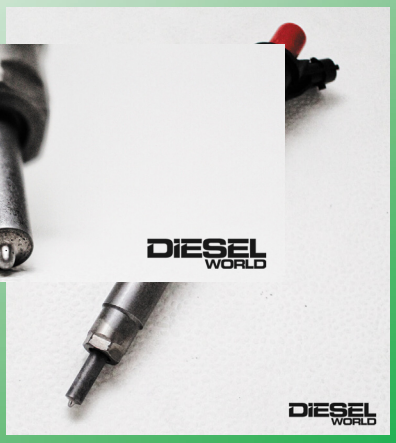

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Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
  - (Plain-)orifice atomizers

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Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
  - (Plain-)orifice atomizers (non-cavitating mode) [1]

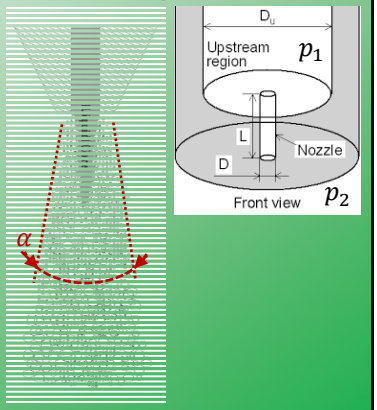
$$V_{\text{inj}} = c_{\text{v}}\sqrt{\frac{2\Delta p}{\rho_l}}$$

$$\frac{\alpha}{2} = \tan^{-1}\left[\frac{4\pi}{A}\left(\frac{\rho_g}{\rho_l}\right)^{0.5}\frac{\sqrt{3}}{6}\right], A = 3 + 0.278\left(\frac{L}{d}\right)$$

$$d_{32} = 133.0\left(\frac{d}{8}\right)\left(\frac{\text{We}_l}{8}\right)^{-0.74}, \text{We}_l = \frac{\rho_l V_{\text{inj}}^2 d}{\sigma}$$

(Rosin-Rammler, $n = 3.5$)

$$\dot{m}_{\text{nozzle}} = c_{\text{d}}\left(A_{\text{nozzle}}\rho_l V_{\text{inj}}\right)$$



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Injector models

- For sprays: called "atomizer models", or " primary breakup models", or …
  - (Plain-)orifice atomizer
  - Pressure-swirl atomizer
  - …
  - See HW#11

Injection algorithm

- Choosing computational parameters:

Injection time step ← $\Delta t_{\text{inj}} = n\Delta t_{\text{L}}$ → Overall Lagrangian time step

N_{inj} → Number of parcels injected per Δt_{inj} for a specific injector

$$\left(\sum_{\text{injectors}} N_{\text{inj}} \frac{FTT}{\Delta t_{\text{inj}}} \leq N_{\max}\right)$$

Flow through time

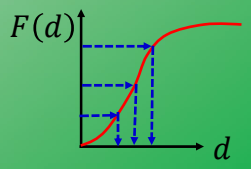
Maximum number of parcels in domain

Injection algorithm

- Choosing computational parameters
- Steps (for each injector):
  1. Generating N_{inj} size samples $d_1, d_2, \ldots, d_{N_{\text{inj}}}$ from the size distribution PDF $f(d)$:
     - Specific random generation methods
     - General "inverse transform method"

$$f(d) \longrightarrow Y = F(d) = \int_0^d f(x)dx \xrightarrow[\text{Analytical or numerical (lookup table)}]{\text{inverse}} d = F^{-1}(Y)$$

$$Y \in U(0,1) \longrightarrow d = F^{-1}(Y)$$



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Injection algorithm

- Choosing computational parameters
- Steps (for each injector):
  1. Generating N_{inj} size samples $d_1, d_2, \ldots, d_{N_{\text{inj}}}$ from the size distribution PDF $f(d)$
  2. Setting other particle properties, given proper statistics:

$$\boldsymbol{x}_p$$
$$\boldsymbol{u}_p = \langle \boldsymbol{u}_p \rangle + \boldsymbol{u}'_p$$
$$\ldots$$

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Injection algorithm

- Choosing computational parameters
- Steps (for each injector):
  1. Generating N_{inj} size samples $d_1, d_2, \ldots, d_{N_{\text{inj}}}$ from the size distribution PDF $f(d)$
  2. Setting other particle properties, given proper statistics
  3. Determining parcel weights:
     - The weights of all samples are equal, otherwise $f(d)$ is violated:

$$w_p = w;\ p = 1, 2, \ldots, N_{\text{inj}}$$

     - w can be computed so as to meet one additional constraint

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Injection algorithm

- Determining w (for each injector):
  - Mass conservation:

$$w = \frac{\overbrace{\left(\dot{m}_p'' A_{\text{inj}}\right)}^{\dot{m}_p} \Delta t_{\text{inj}}}{\sum_{p=1}^{N_{\text{inj}}} m_p}$$

  - Number conservation:

$$w = \frac{\left(\dot{m}_p'' A_{\text{inj}}\right) \Delta t_{\text{inj}}}{\frac{\pi}{6} \rho_p \langle d_p^3 \rangle N_{\text{inj}}}$$

- If $\dot{m}_p''$ is not given directly, it can be approximated by:

$$\dot{m}_p'' \simeq n_M u_{p,\perp} \simeq \frac{\pi}{6} \rho_p \langle d_p^3 \rangle \overbrace{n}^{\text{number concentration}} u_{p,\perp} \simeq \frac{\pi}{6} \rho_p \langle d_p^3 \rangle \dot{n}_p''$$

mass concentration; Particle velocity normal to boundary; Number flow rate

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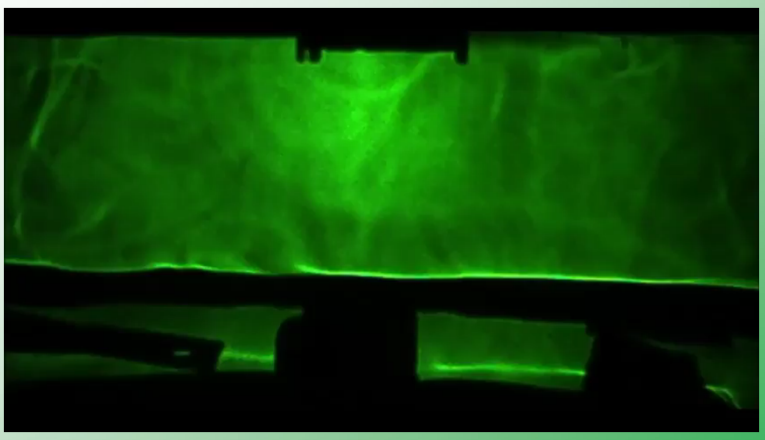
Case study #4: Spray-wall impact



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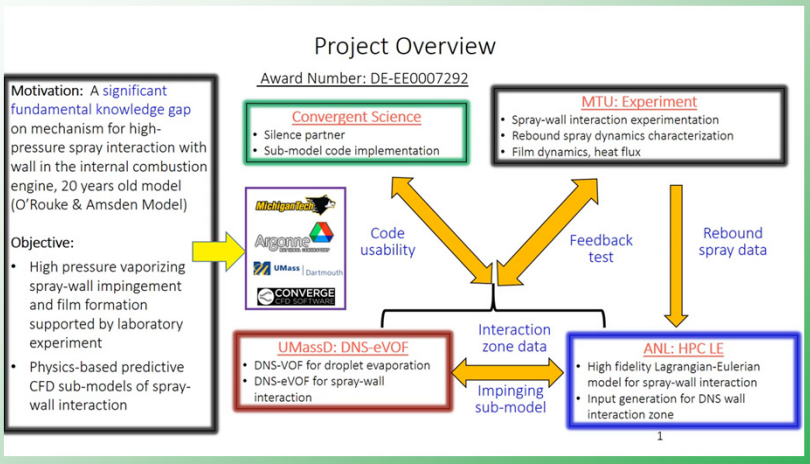
Case study #4: Spray-wall impact



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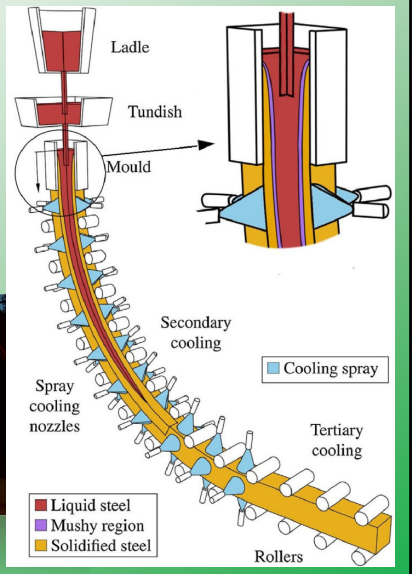
Case study #4: Spray-wall impact

- **Applications:**
  - **Spray cooling**

Continuous casting ▼ ►



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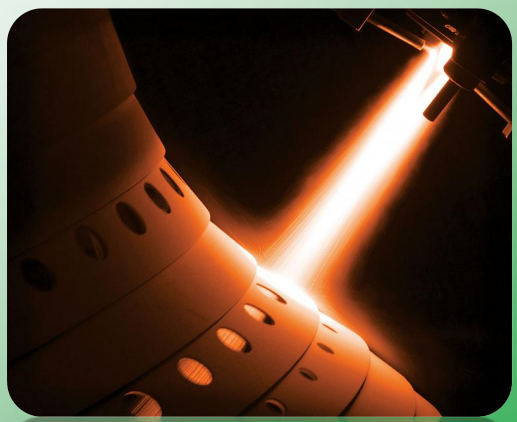
Case study #4: Spray-wall impact

- **Applications:**
  - **Spray cooling**
  - **Thermal spray coating**



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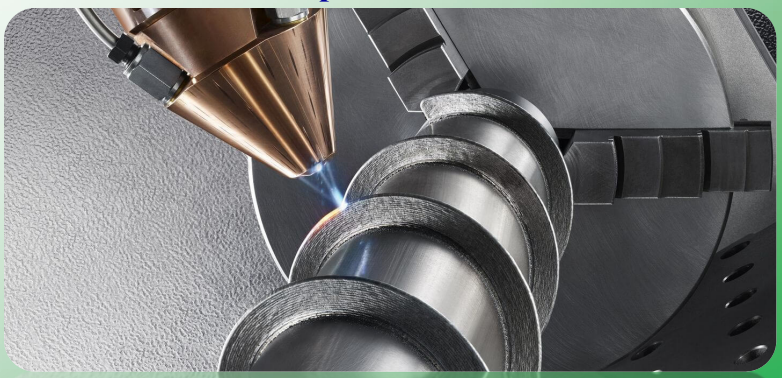
Case study #4: Spray-wall impact

- Applications:
  - Spray cooling
  - Thermal spray coating
  - Laser metal deposition



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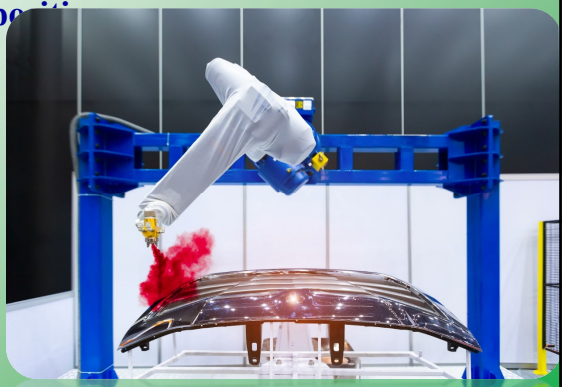
Case study #4: Spray-wall impact

- Applications:
  - Spray cooling
  - Thermal spray coating
  - Laser metal depo
  - Spray painting



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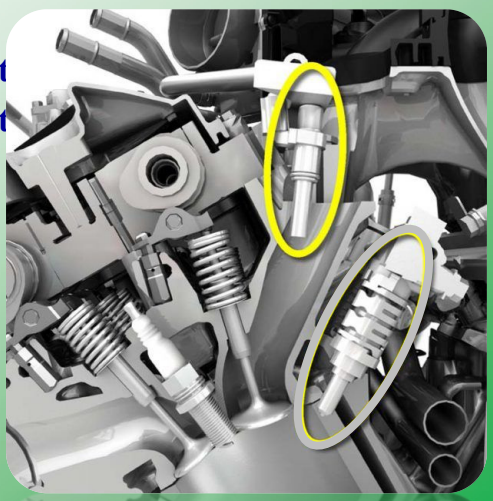
Case study #4: Spray-wall impact

- **Applications:**
  - **Spray cooling**
  - **Thermal spray coat**
  - **Laser metal deposit**
  - **Spray painting**
  - **Port fuel injection**
  - **…**



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Case study #4: Spray-wall impact

- **Problem definition:**

$H_d = 10\ cm$

$L_d = 50\ cm$

Injector specification:

Type: Plain-orifice injector

Liquid: Water

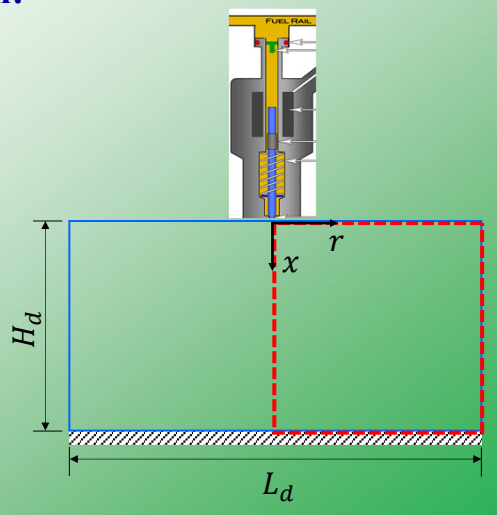
$D = 500\ \mu m$

$L/D = 10$

$\Delta p = 1\ MPa$

$c_v = 0.8,\ c_d = 0.6$

$\frac{\alpha}{2} = 20$ deg



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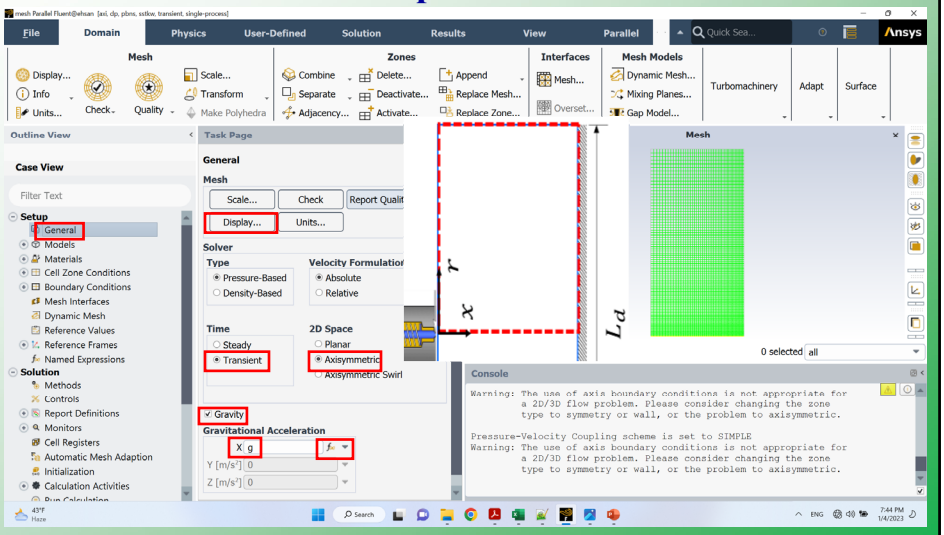
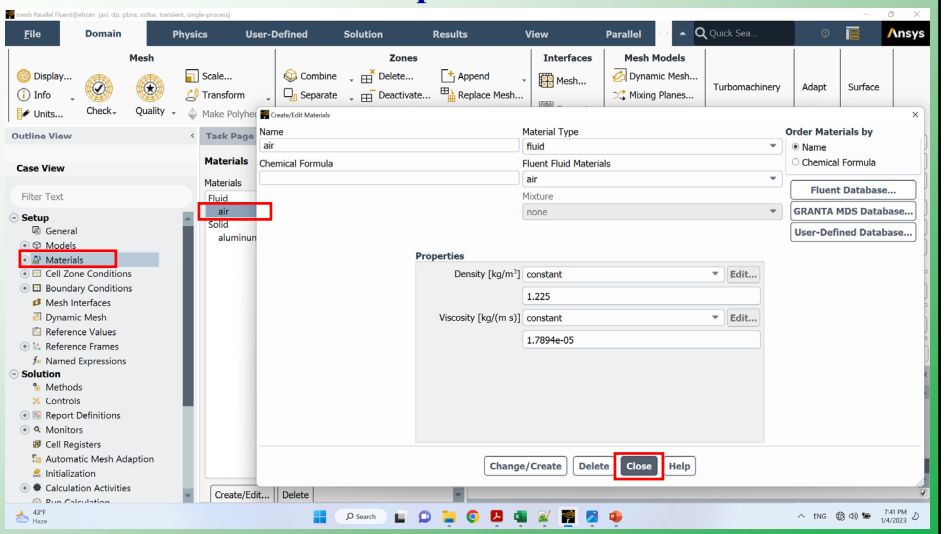
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: General**



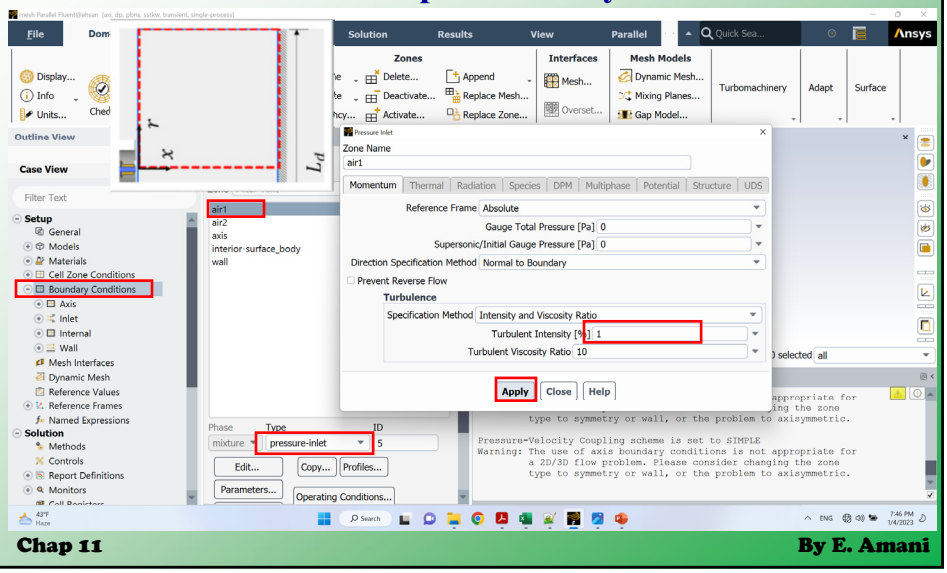
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Materials**



Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Boundary Conditions**



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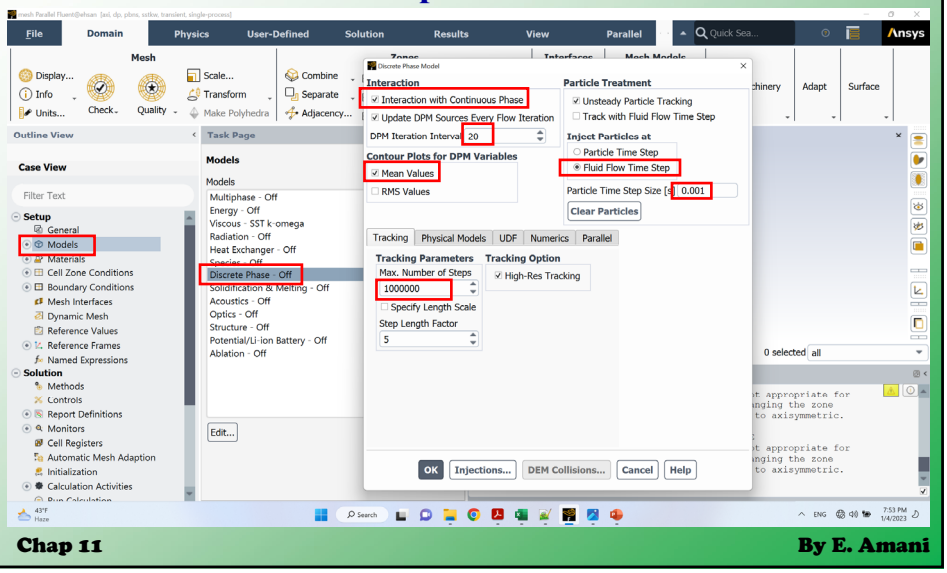
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Models**



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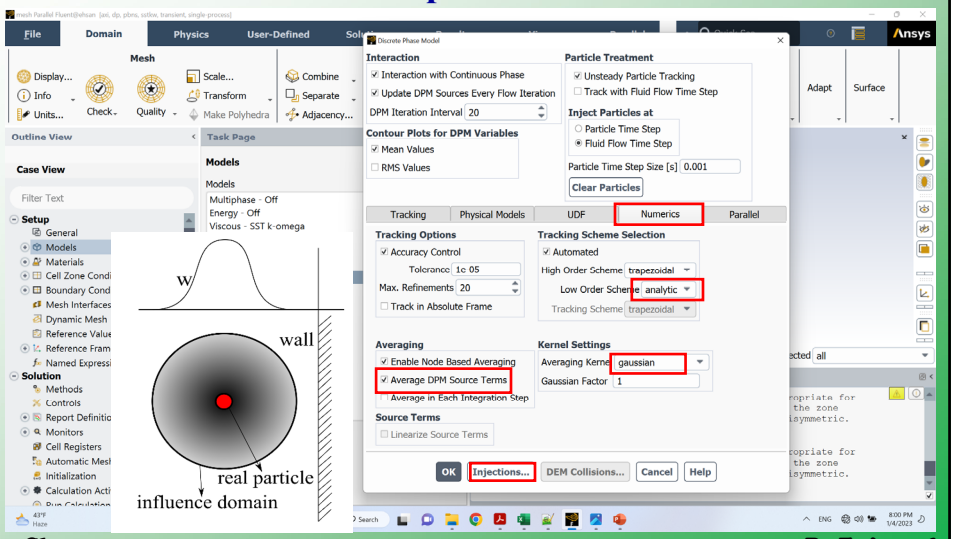
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Models**



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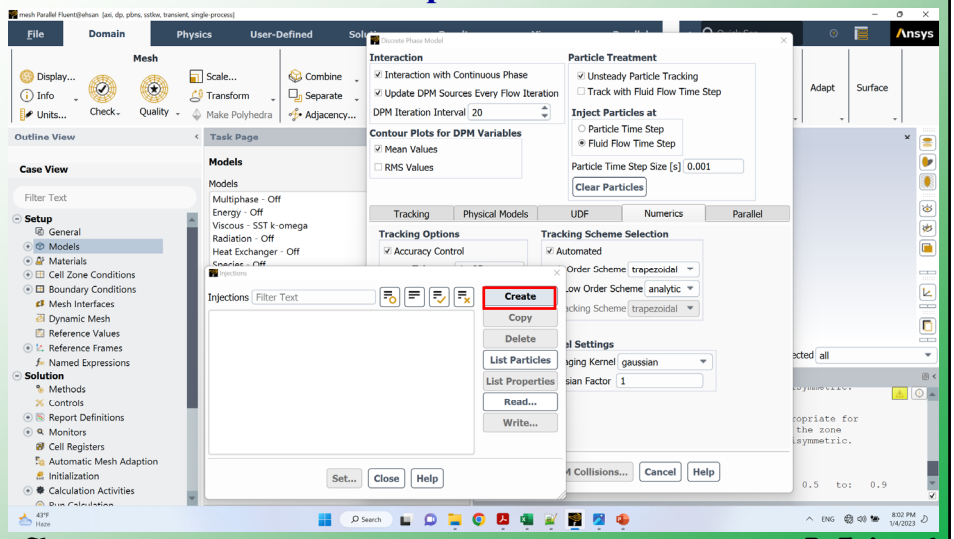
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Models**



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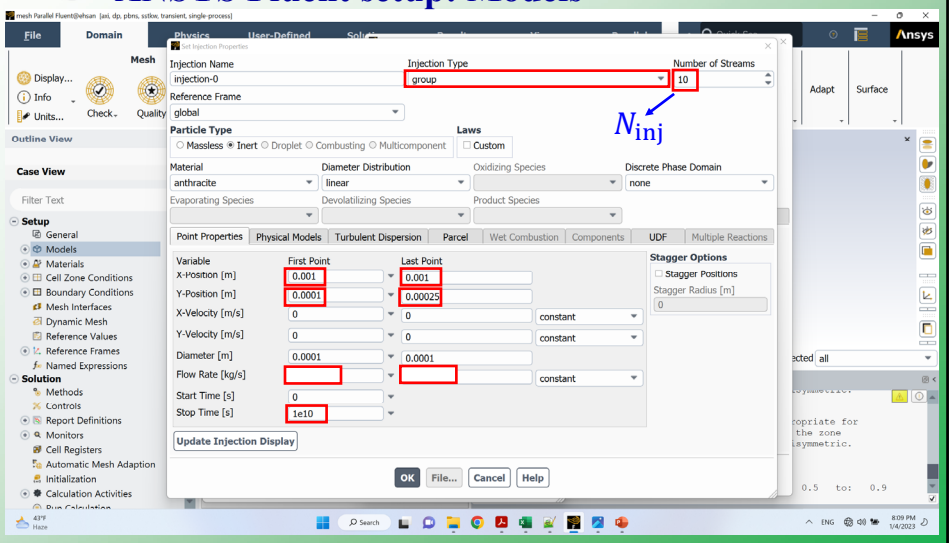
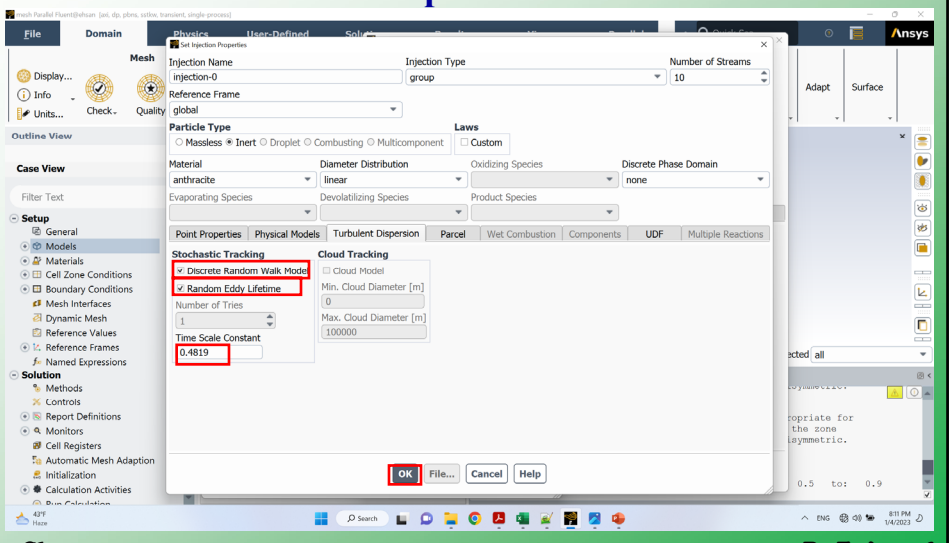
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Models**



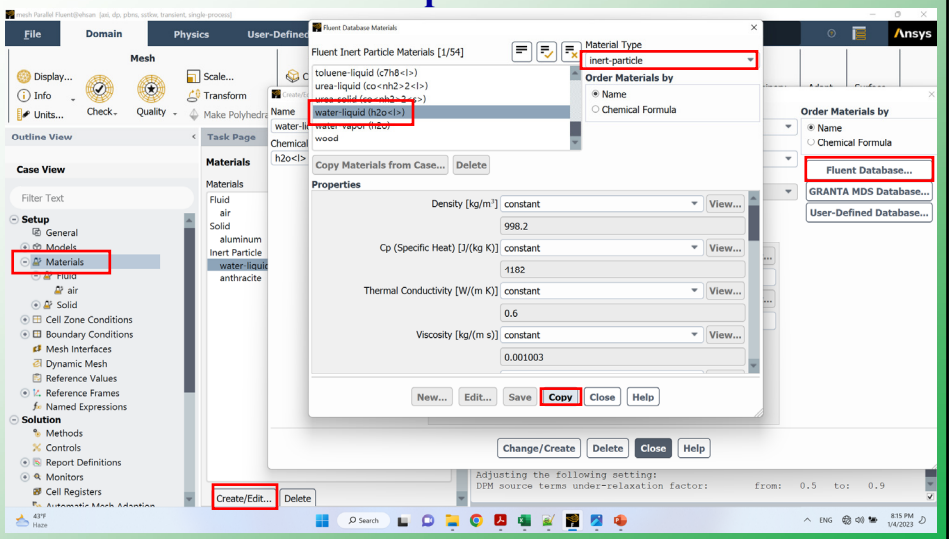
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Models**



Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Materials**



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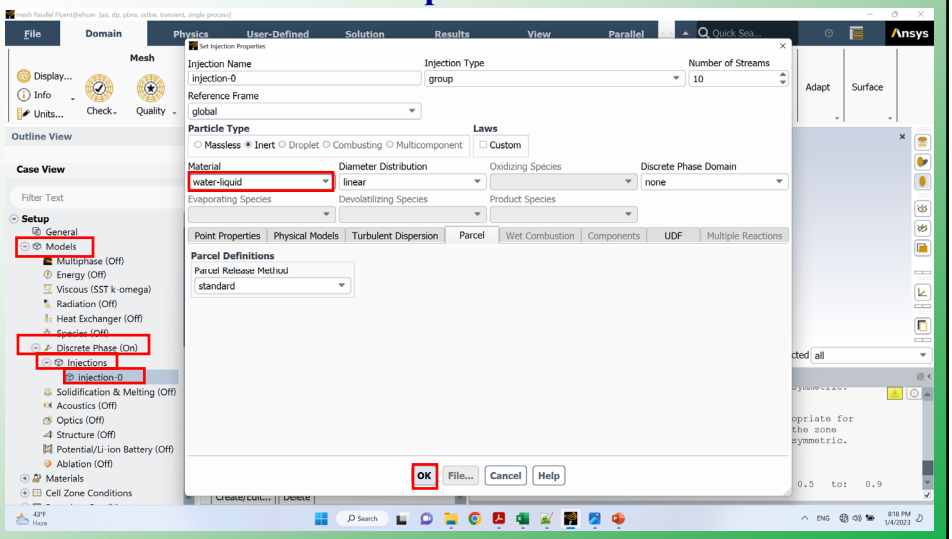
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Materials**



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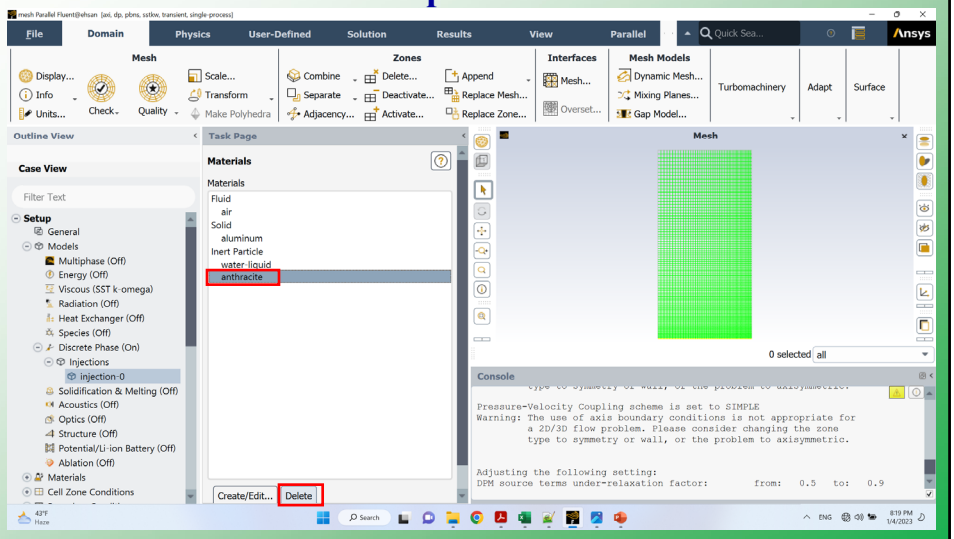
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Materials**



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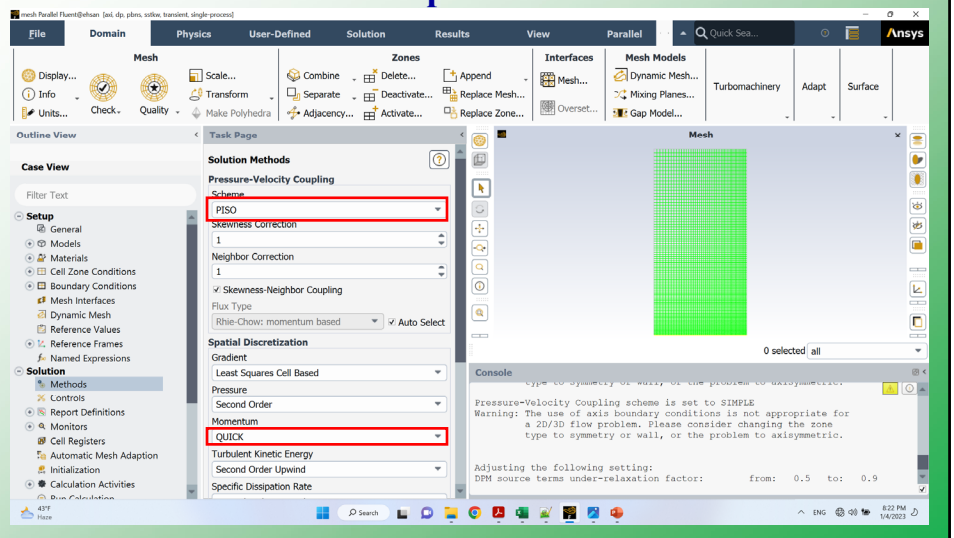
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Solution**



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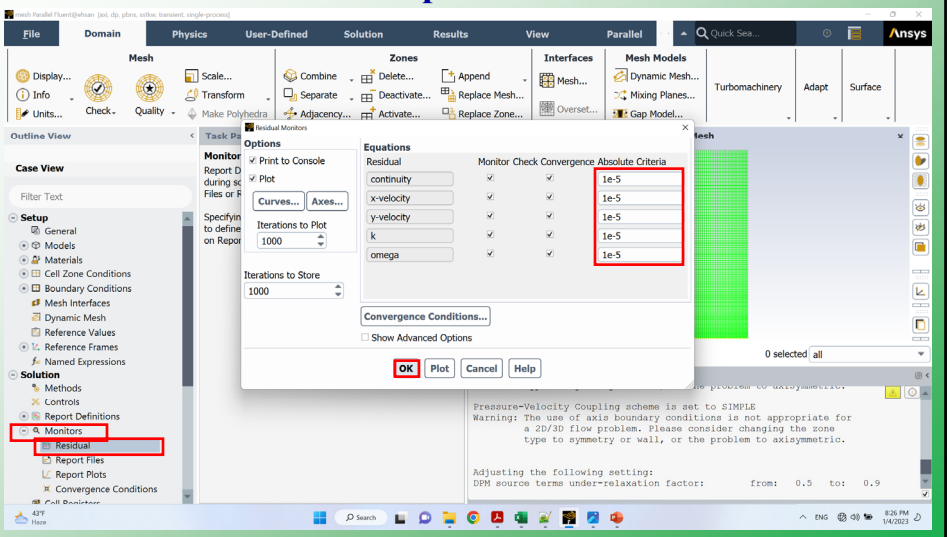
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Monitors**



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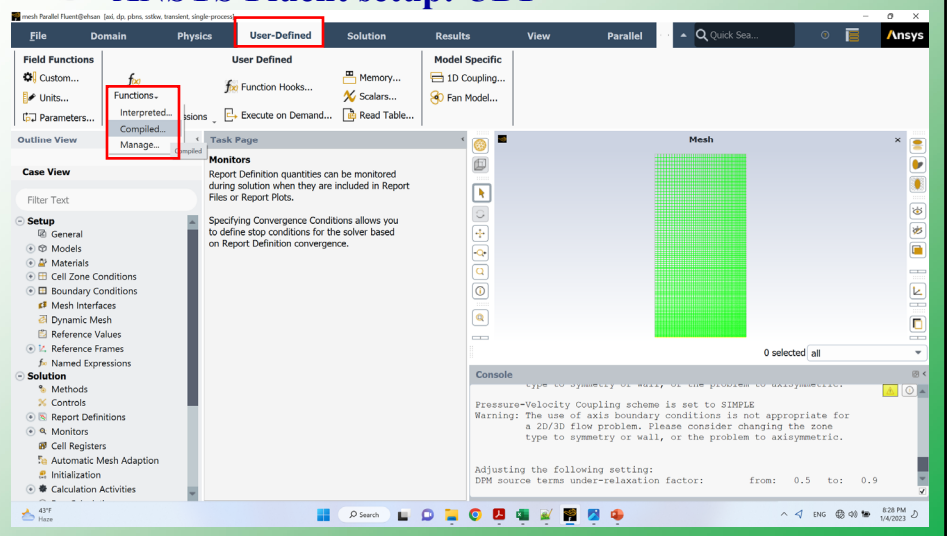
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



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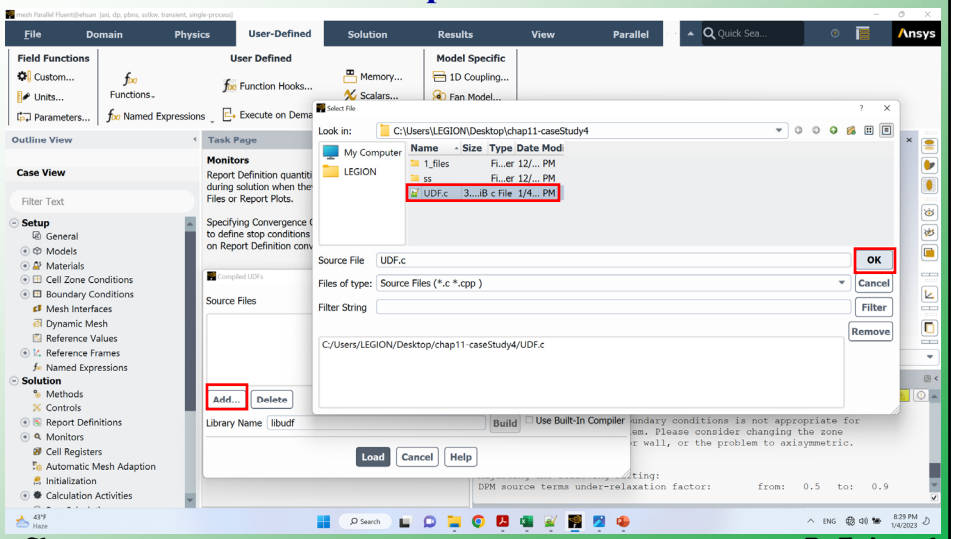
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



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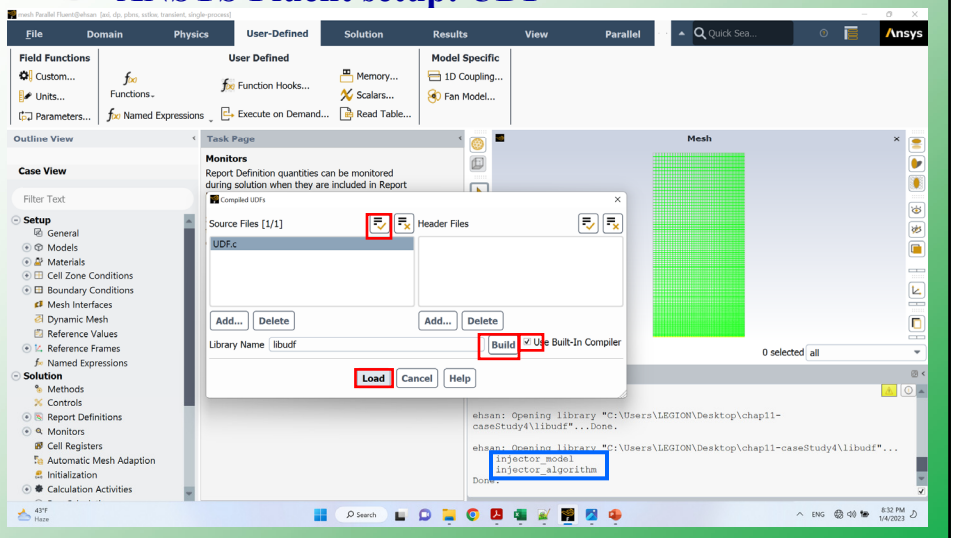
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



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Injection modeling hierarchy

Simpler initial condition

Direct inputs

Injector specification

ΔP_{inj}, Geometry (d_{nozzle}, L), …

Injector models

Empirical correlations, stability analysis, …

Injection statistics

$\dot{m}_p$ or n_p or C_{Mp}

$f(d)$ or $(\bar{d}, \sigma, \ldots)$

f_{du} or …

…

Computational parameters

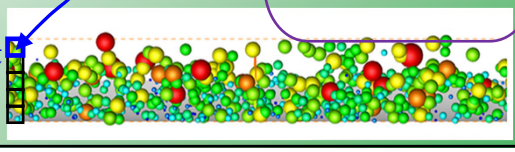
Δt_{inj}, N_{inj}

Stochastic processes

Injection algorithm

$x_p, u_p, d_p, \ldots, w_p$

inlet



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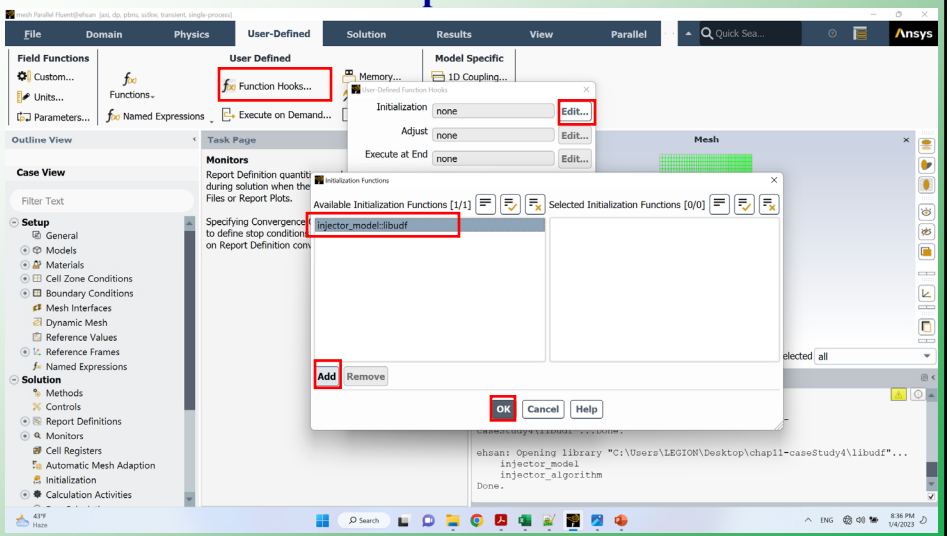
Case study #4: Spray-wall impact

- ANSYS Fluent setup: UDF



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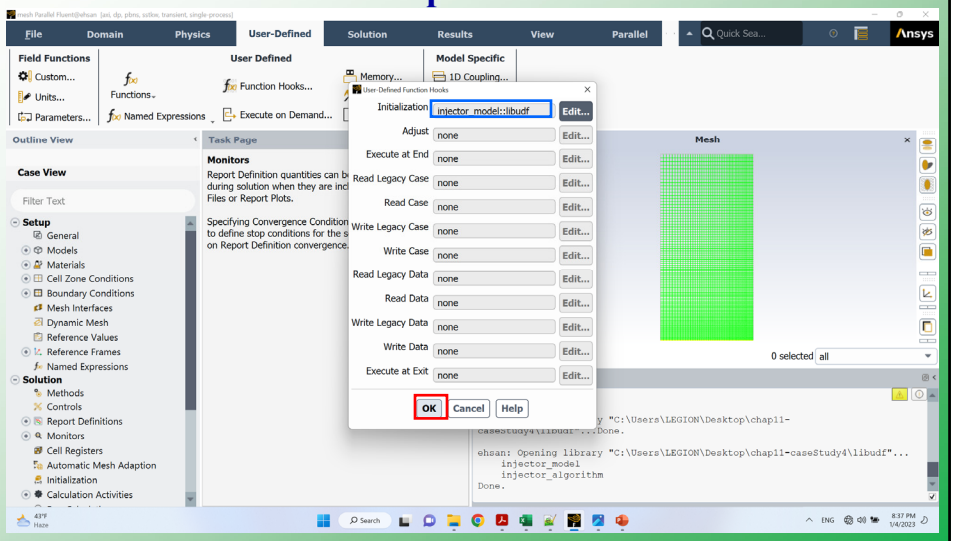
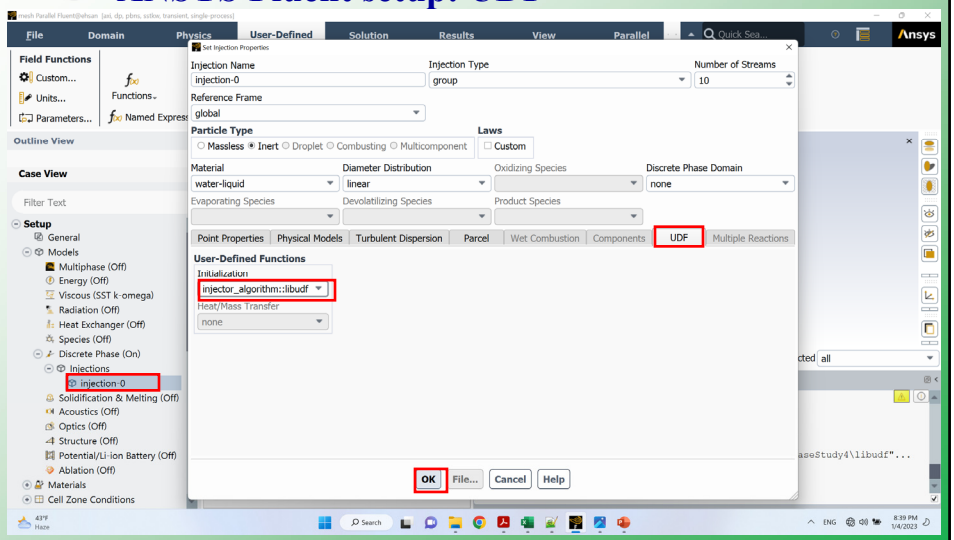
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



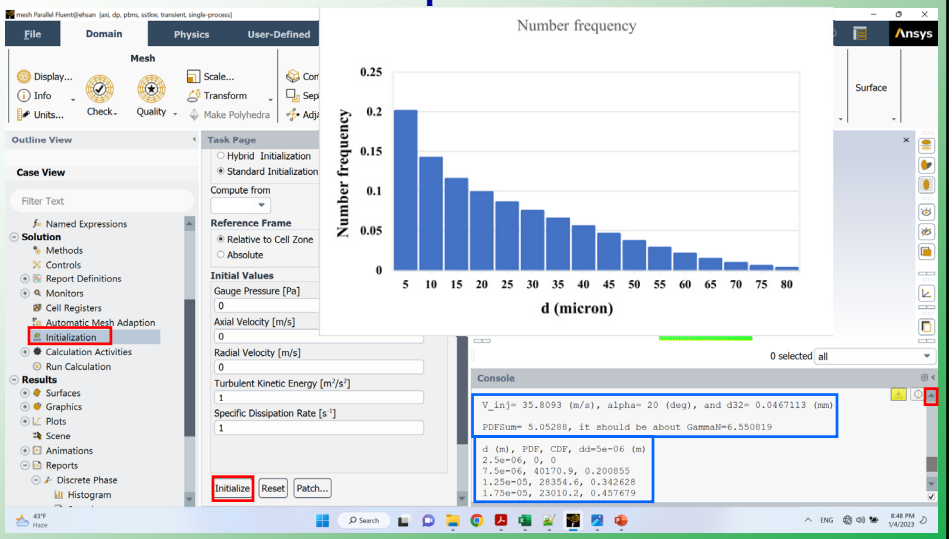
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Initialization**



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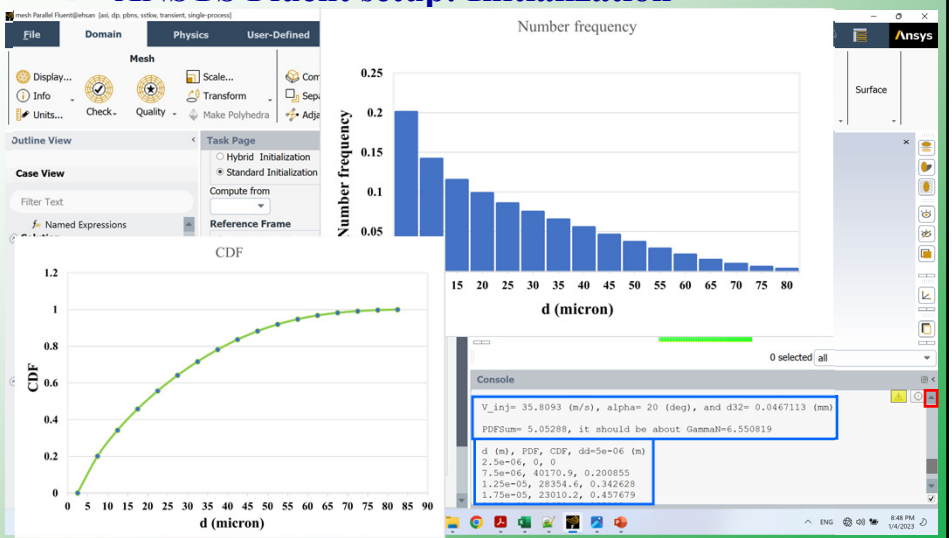
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Initialization**



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Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

UDF.c

```
/*****************************************************************/
/*                                                               */
/* NSMF-chap11-VOF                                               */
/* By Dr. Ehsan Amani                                            */
/* First version: January 2023                                   */
/*                                                               */
/*****************************************************************/

//Headers
#include "udf.h"
#include "dpm.h"
#include "surf.h"
#include "random.h"


//INPUTS
#define dP 1.e6 // Pa
#define Cv 0.8
#define Cd 0.6
#define sIndex 3.5
#define rho_l 998.2 // kg/m3
#define rho_g 1.225 // kg/m3
#define sigma 0.0728 // N/m
#define Ndata 16
#define D 500.e-6 // m
#define alphad 20 //deg
#define L 5.e-3 // m
#define dT_inj 0.005 //s
#define dmin 2.5e-6 //m
#define dmax 82.5e-6 //m


void RR_PDFcalc(double sI, double delta, double dmi, double dma, double d[], double PDF[], double* dd);
void CDF_calc(double d[], double PDF[], double dd, double CDF[]);
double ITM_sample(void);

double d[Ndata+1]={0.}, PDF[Ndata+1]={0.}, CDF[Ndata+1]={0.};
double dd=0., V_inj=0., alpha=0., mdot_inj=0.;
```


Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

UDF.c

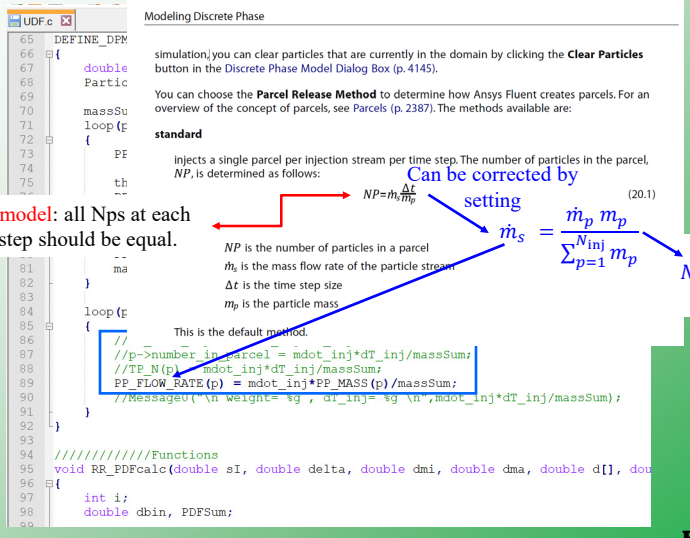
```
//////////////FLUNT UDF Macros
DEFINE_INIT(injector_model, domain)
{
    double A, We, d32, delta;
    int i;

    A=3.0+0.28*L/D;
    V_inj=Cv*sqrt(2*dP/rho_l);
    mdot_inj=Cd*(M_PI/4*D*D)*rho_l*V_inj;
    We=rho_l*pow(V_inj,2.)*(D/8)/sigma;
    //alpha=atan(4*M_PI/A*sqrt(3*ro_g/ro_l)/6);
    alpha=alphad*M_PI/180;
    d32=133.0*(D/8)*pow(We,-0.74);
    delta=1.2726*d32;

    Message0("\n V_inj= %g (m/s), mdot_inj= %g (g/s), alpha= %g (deg), and d32= %g (mm) \n",V_inj,md

    RR_PDFcalc(sIndex, delta, dmin, dmax, d, PDF, &dd);
    CDF_calc(d, PDF, dd, CDF);
    Message0("\n d (m), PDF, CDF, dd=%g (m) ", dd);
    for (i=0; i<(Ndata+1); i++)
    {
        Message0("\n %g, %g, %g ",d[i],PDF[i],CDF[i]);
    }
}
```

Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**



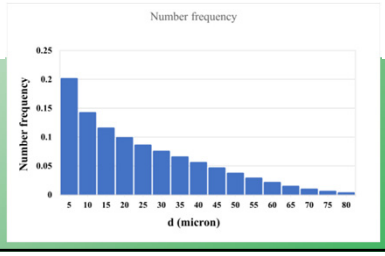
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

UDF.c

```
94  ////////////Functions
95  void RR_PDFcalc(double sI, double delta, double dmi, double dma, double d[], double PDF[], double* dd)
96  {
97      int i;
98      double dbin, PDFSum;
99
100     d[0]=dmi;
101     PDF[0]=0;
102     *dd=(dma-dmi)/Ndata;
103     PDFSum=0.;
104     for (i=1; i<(Ndata+1); i++)
105     {
106         d[i]=d[i-1]+(*dd);
107         dbin=d[i-1]+(*dd)/2;
108         PDF[i]=sI/delta*pow(dbin/delta,sI-4)*exp(-pow(dbin/delta,sI)); //1./GammaN=0.15265
109         PDFSum+=PDF[i]*(*dd);
110     }
111     Message0("\n PDFSum= %g, it should be about GammaN=6.550819 \n",PDFSum);
112     for (i=1; i<(Ndata+1); i++) //normalization
113     {
114         PDF[i]/=PDFSum;
115     }
116 }
```

$$f(d) = \frac{1}{\Gamma}\frac{s}{\delta}\left(\frac{d}{\delta}\right)^{s-4} \exp\left[-\left(\frac{d}{\delta}\right)^{s}\right]$$



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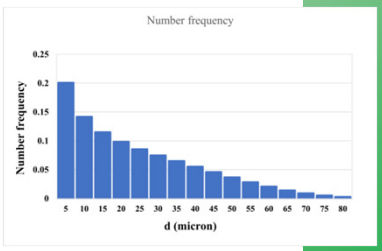
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

```
117
118 //Inverse transform method
119 void CDF_calc(double d[], double PDF[], double dd, double CDF[])
120 {
121     int i;
122
123     CDF[0]=0;
124     for (i=1; i<(Ndata+1); i++)
125     {
126         CDF[i]=CDF[i-1]+dd*PDF[i];
127     }
128 }
129
130 double ITM_sample(void)
131 {
132     double y, w;
133     int i;
134
135     y= cheap_uniform_random();
136     for (i=1; i<(Ndata+1); i++)
137     {
138         if (y<=CDF[i]) break;
139     }
140     w=(CDF[i]-y)/(CDF[i]-CDF[i-1]);
141
142     return w*d[i-1]+(1.-w)*d[i];
143 }
```

$$F(d) = \int_0^d f(d')dd'$$



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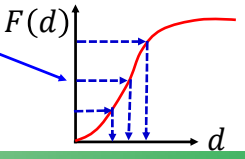
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: UDF**

```
117
118  //Inverse transform method
119  void CDF_calc(double d[], double PDF[], double dd, double CDF[])
120  {
121      int i;
122
123      CDF[0]=0;
124      for (i=1; i<(Ndata+1); i++)
125      {
126          CDF[i]=CDF[i-1]+dd*PDF[i];
127      }
128  }
129
130  double ITM_sample(void)
131  {
132      double y, w;
133      int i;
134
135      y= cheap_uniform_random();
136      for (i=1; i<(Ndata+1); i++)
137      {
138          if (y<=CDF[i]) break;
139      }
140      w=(CDF[i]-y)/(CDF[i]-CDF[i-1]);
141
142      return w*d[i-1]+(1.-w)*d[i];
143  }
```

$$Y \in U(0,1) \longrightarrow d = F^{-1}(Y)$$



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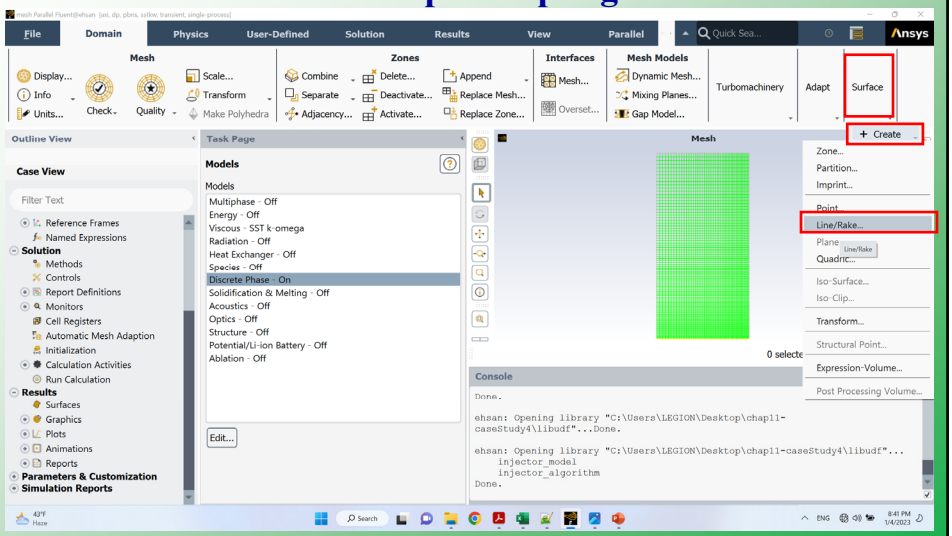
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Sampling**



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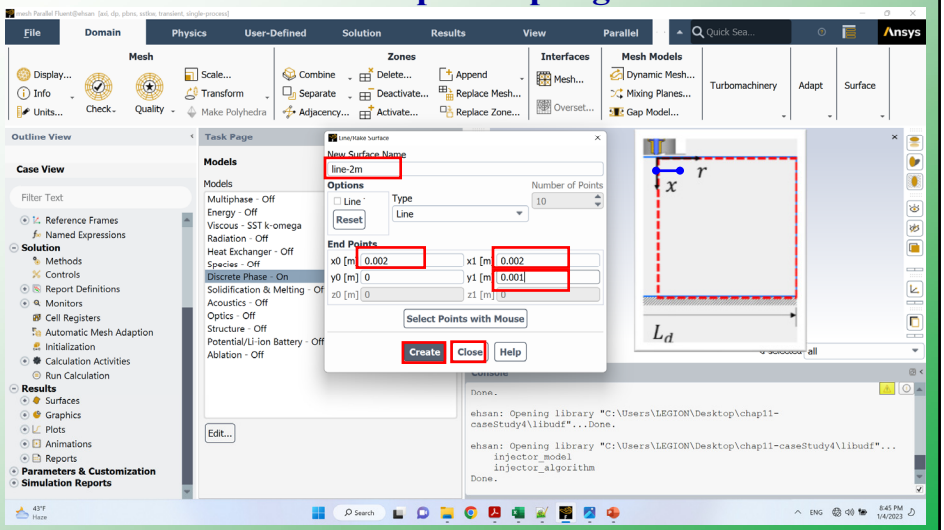
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Sampling**



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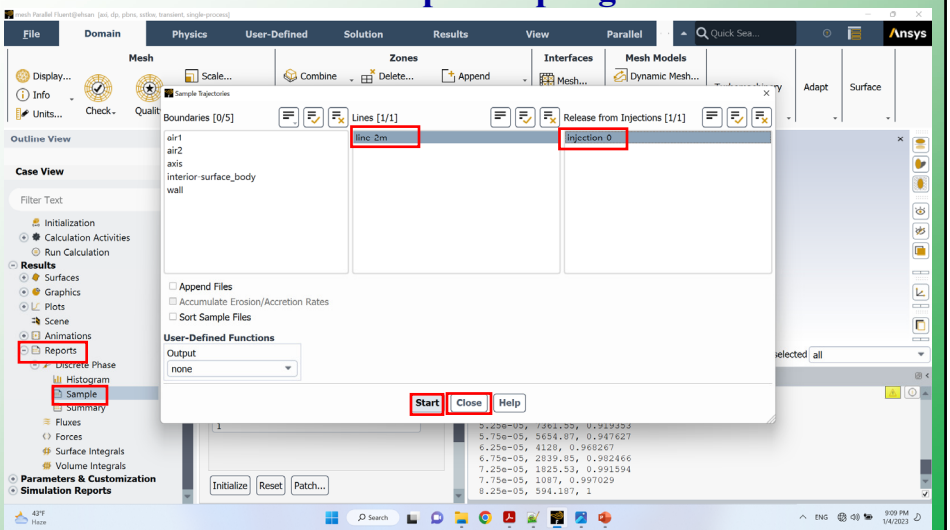
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Sampling**



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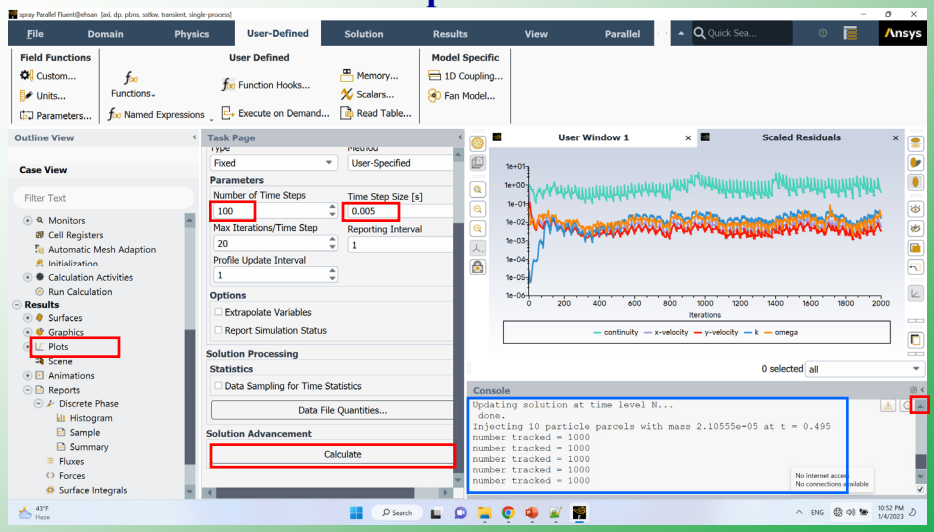
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Run**



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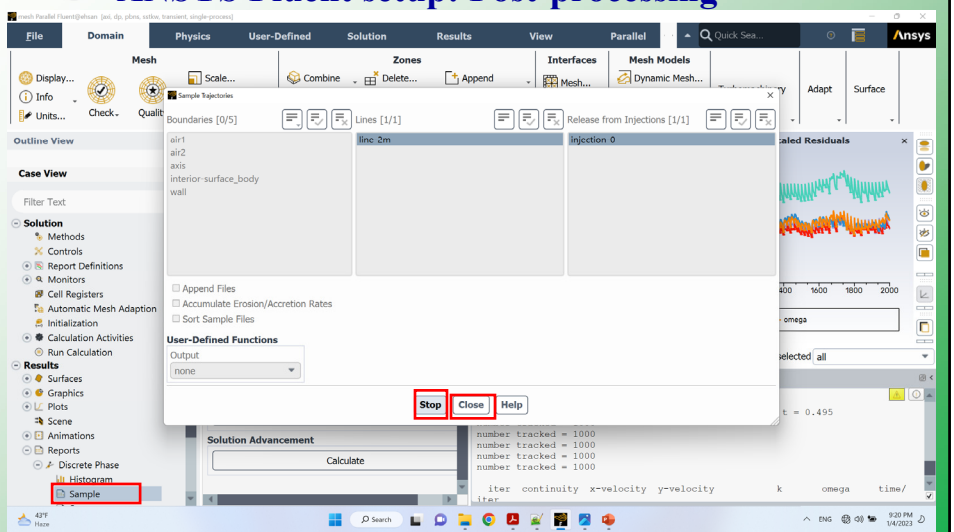
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Post-processing**



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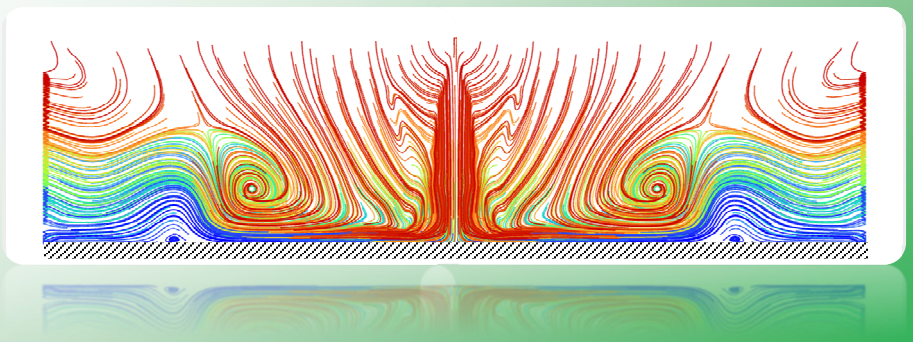
Case study #4: Spray-wall impact

- **ANSYS Fluent setup: Post-processing**



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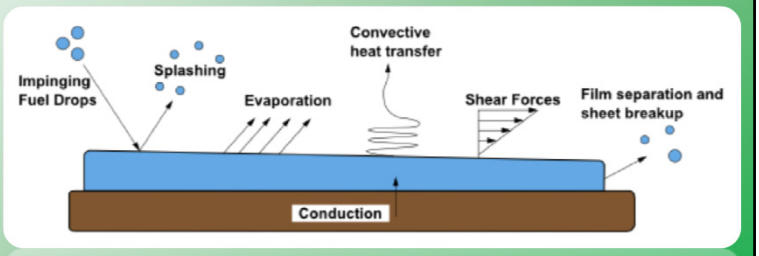
Boundary conditions

- Droplet-wall impact models
  - Stick
  - Reflect
  - Wall-jet (hot walls with no film)
  - Wall-film, e.g., you can see Ref. [2]
  - …



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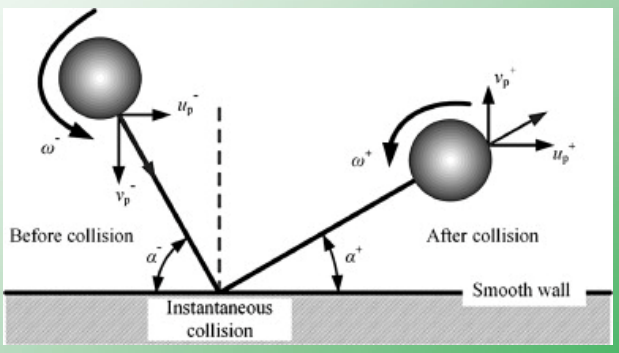
Boundary conditions

- Solid-particle-wall impact models
  - Regular bouncing



$$m_2 \to \infty, r_2 \to \infty$$

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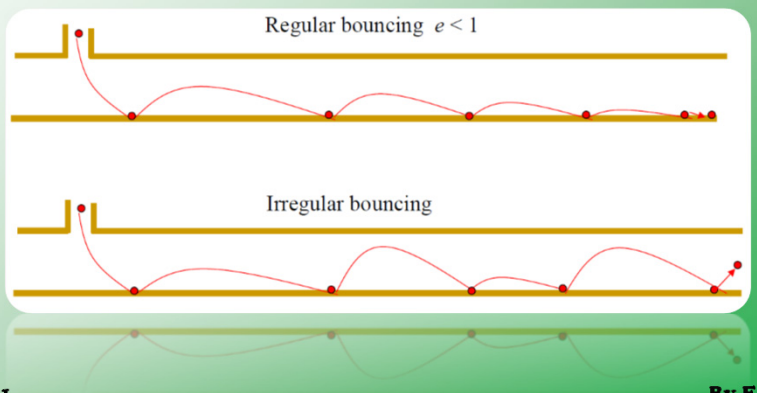
Boundary conditions

- Solid-particle-wall impact models
  - Regular bouncing
  - Irregular bouncing



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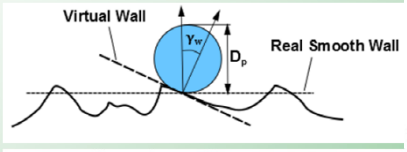
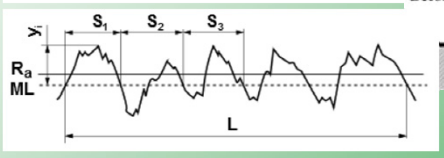
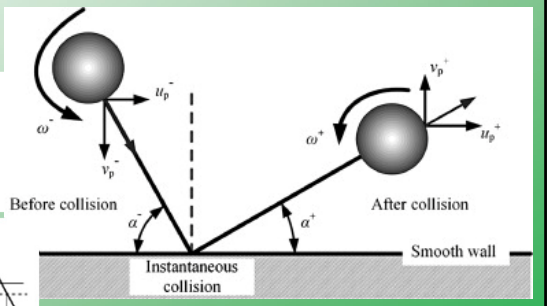
Boundary conditions

- Solid-particle-wall impact models
  - Regular bouncing
  - Irregular bouncing

$$\alpha_{\text{impact}} = \alpha^{-} + \alpha_{\text{W}}$$



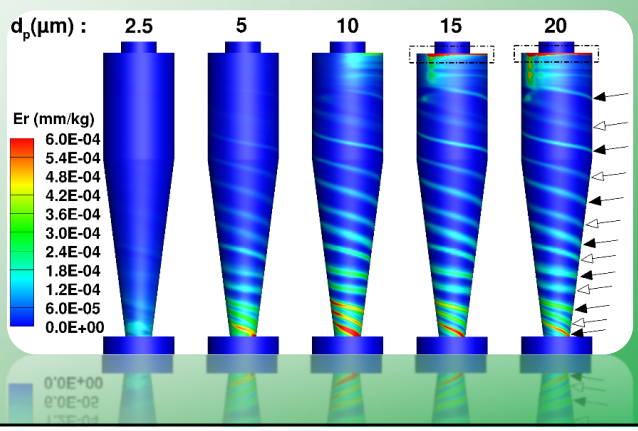




(See HW#11)

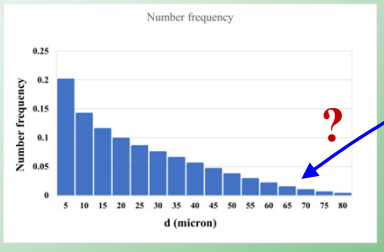
Post-processing

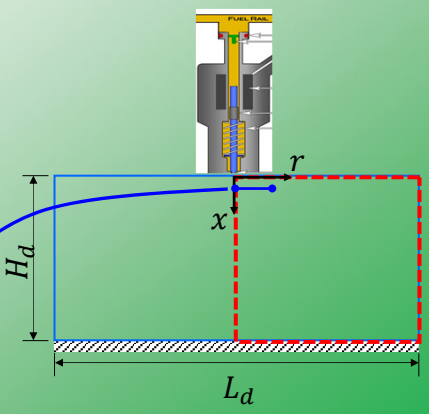
- Erosion
  - Solid particles
  - Irregular bouncing, e.g., you can see Ref. [3]



Hands-on practice

- HW#11
  - ✓ Processing the samples recorded near the nozzle and check the PDF of injected particles
  - ✓ …





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References

1. Ashgriz, Nasser, ed. Handbook of atomization and sprays: theory and applications. Springer Science & Business Media, 2011.
2. Asgari, Behrad, and Ehsan Amani. An improved spray-wall interaction model for Eulerian-Lagrangian simulation of liquid sprays. International Journal of Multiphase Flow 134 (2021): 103487.
3. Tofighian, H., E. Amani, and M. Saffar-Avval. "A large eddy simulation study of cyclones: The effect of sub-models on efficiency and erosion prediction." Powder Technology 360 (2020): 1237-1252.

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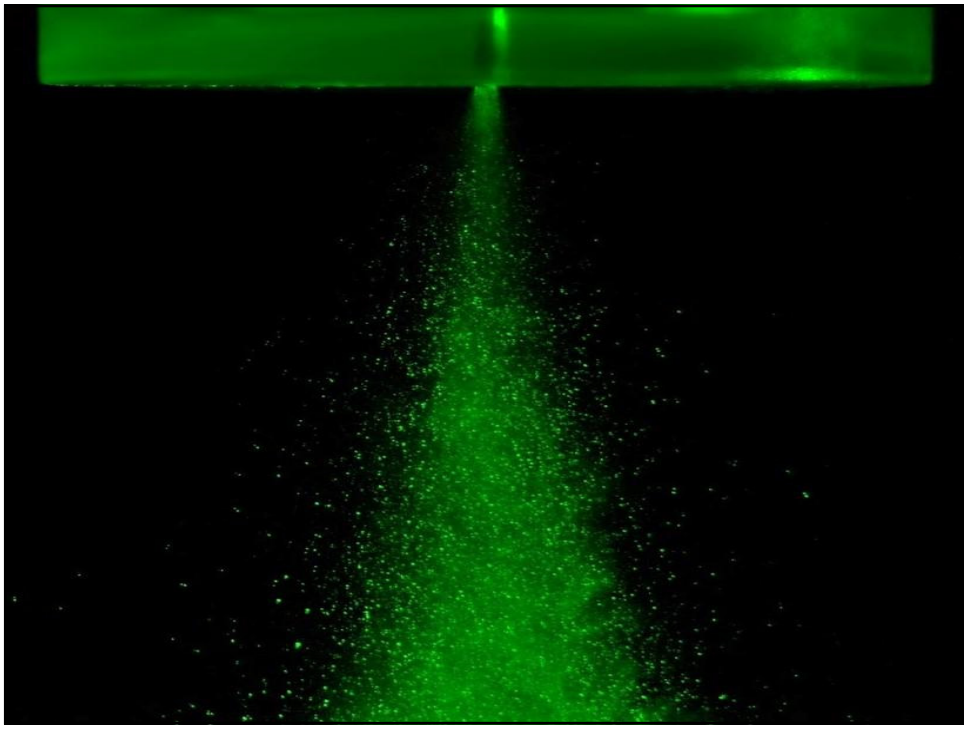

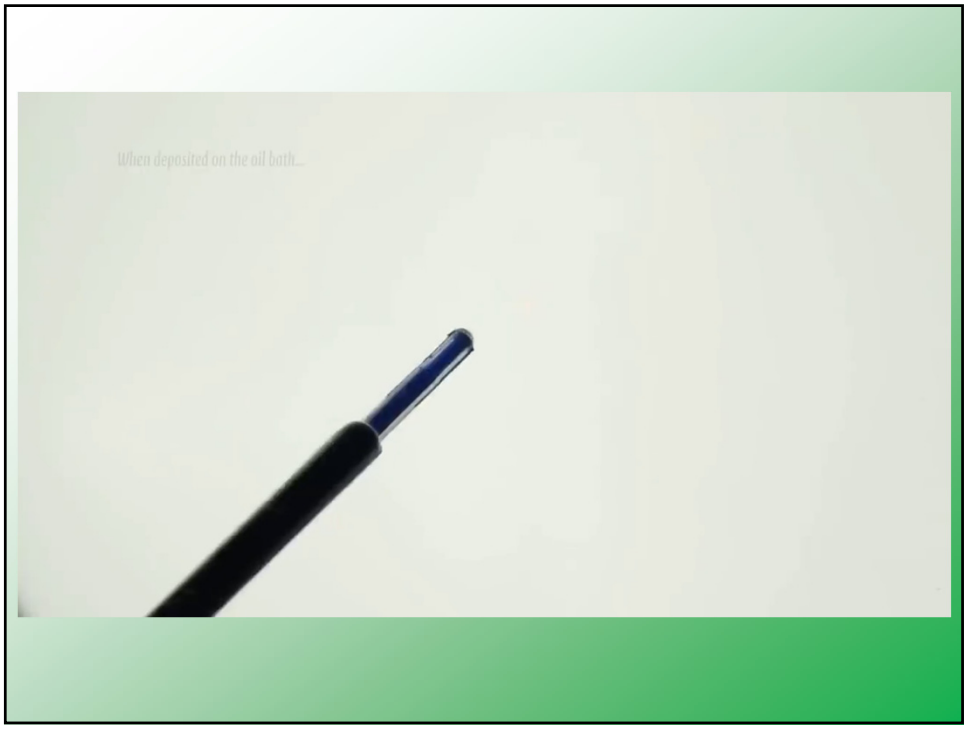
When deposited on the oil bath...