Modelling of test case particle-laden jet with NEPTUNE_CFD

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I. Introduction
**Thesis context**

**Thesis subject:** Modelling of pressurized jet loaded with nanoparticles.

- Rapidly increase of use of nanotechnology in industrial process
- Application in safety management

**Collaboration between:**
- **INERIS:** Institut National de l’Environnement Industriel et des Risques
- **IMFT:** Institut de Mécanique des Fluides de Toulouse

Accidental configuration: leakage of conveying pipe of nanoparticle

Atmospheric dispersion model in the far field

CFD Study in the near field

Source term

Thesis started day : January 05th 2015
Phenomena involved in nanoparticle dispersion:

Additional physical modelling of particulate jet:
- Drag
- Influence of particles on fluid turbulence
- Collision between particles
- Gravity, etc...

Numerical simulation tools currently used:
- **NEPTUNE_CFD V2.0** supported by CEA (Commissariat à l’Energie Atomique), EDF (Electricité de France), IRSN (Institut de Radioprotection et de Sûreté Nucléaire) and AREVA which use Euler multifluid approach – RANS.
- **Code_Saturne v4.0** developed by EDF which uses Euler – Lagrange approach – RANS/LES.

**Thesis approach:**
- Numerical simulation of **microparticle** dispersion before numerical simulation of **nanoparticle** dispersion
- Implementation of modelling of Brownian motion and agglomeration in numerical simulation tools
Test case

Aim of the test case: Evaluation of numerical simulation tool NEPTUNE_CFD V2.0.

4 flow configurations:

- Single phase flow of gas
- Two-phase flow with 25 μm particles
- Two-phase flow with 70 μm particles
- Two-phase flow with binary mixture (25 μm particles and 70 μm particles)

Available experimental data provied by the Workshop Committee:

- Velocity of gas and particulate phases at nozzle exit and at centre line
- Velocity of particulate phase at axial positions of X/D=5, 10 and 15
  - $D$: nozzle diameter
  - $Re \approx 8,400$

II. Theoretical models used by NEPTUNE_CFD
Governing equations

Unsteady eulerian multifluid approach for gas phase and particulate phase[1]:

- **Continuous phase**: derived from local instant conservation equations in single-phase flow by density-weighted averaging (Favre averaging)

- **Particulate phase**: derived in the frame of the kinetic theory of granular media based on a statistical approach using a Probability Density Function (PDF)

Balance equations are solved for each phase:

- **Mass balance**
  \[
  \frac{\partial}{\partial t} \alpha_k \rho_k + \frac{\partial}{\partial x_j} \alpha_k \rho_k U_{k,j} = 0
  \]

- **Momentum balance**
  \[
  \alpha_k \rho_k \left[ \frac{\partial U_{k,i}}{\partial t} + U_{k,j} \frac{\partial U_{k,i}}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[ -\alpha_k \rho_k \left\langle u_{k,i}^\prime, u_{k,j}^\prime \right\rangle \right] + \alpha_k \rho_k g_i + \alpha_k \frac{\partial P_g}{\partial x_i} + \sum_{k'=g,p} I_{k' \rightarrow k,i}
  \]

  - **Momentum exchange of gas-particles and particles-particles phases**
    \[ I_{k' \rightarrow k,i} \]
  
  \[
  k = g : \text{gas phase} \\
  k = p : \text{particulate phase}
  \]

Closure models for momentum exchange

Momentum transfer between gas and particulate phase [1]

\[ I_{g \rightarrow p, i} = -\frac{\alpha_p \rho_p}{\tau_{gp}^F} V_{r,i} \]

Drag model

Relaxation time of particles \( \tau_{gp}^F \)

\[ \frac{1}{\tau_{gp}^F} = \frac{3 \rho_g}{4 \rho_p d_p} \langle |v_r| \rangle C_d \]

Mean relative velocity of gas-particle

\[ V_{r,i} = U_{p,i} - U_{g,i} - V_{d,i} \]

Wen and Yu model[2] for \( C_d \)

\[ C_d = \begin{cases} 
24 \left( 1 + 0.15 \text{Re}_p^{0.687} \right) \alpha_g^{-1.7} & \text{Re}_p < 1000 \\
0.44 \alpha_g^{-1.7} & \text{Re}_p \geq 1000 
\end{cases} \]

Closure models for momentum exchange

Momentum transfer between particles [1]

\[ I_{q \rightarrow p,i} = -\frac{m_p m_q}{m_p + m_q} \frac{1 + e_c}{2} n_p \frac{U_{p,i} - U_{q,i}}{\tau_{pq}} \left[ \frac{H_1(z)}{e_c} \right] \]

\[ \frac{1}{\tau_{pq}^c} = \pi n_q d_{pq}^2 g_r \]

Collision characteristic time

Particle mean relative velocity at impaction

\[ g_r = \sqrt{\frac{16}{\pi} \frac{2}{3} q_r + U_{pq,i} U_{pq,i}} \]

Particle mean agitation

\[ q_r = \frac{1}{2} \left( q_p^2 + q_q^2 \right) \]

Particle mean relative velocity

\[ U_{pq,i} = U_{p,i} - U_{q,i} \]

Model approximation

\[ H_1(z) = \frac{8 + 3z}{6 + 3z} \]

Model parameter

\[ z = \frac{3U_{pq,i} U_{pq,i}}{8q_r} \]

Coefficient of restitution

\[ e_c = 0.9 \text{ For the test case} \]

Closure models for turbulence

Fluid turbulence model[1]  \( k - \varepsilon \)

*Turbulence created by wake of particulate phase is not considered.

\[
\begin{align*}
\alpha_g \rho_g \left[ \frac{\partial k}{\partial t} + U_{g,j} \frac{\partial k}{\partial x_j} \right] &= \frac{\partial}{\partial x_j} \left[ \alpha_g \rho_g \frac{\nu_g'}{\sigma_k} \frac{\partial k}{\partial x_j} \right] - \alpha_g \rho_g \varepsilon - 2k \frac{\partial U_{g,i}}{\partial x_j} + \sum_p \Pi^k_{p \to g} \\
\alpha_g \rho_g \left[ \frac{\partial \varepsilon}{\partial t} + U_{g,j} \frac{\partial \varepsilon}{\partial x_j} \right] &= \frac{\partial}{\partial x_j} \left[ \alpha_g \rho_g \frac{\nu_g'}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x_j} \right] - \alpha_g \rho_g \frac{\varepsilon}{k} \left[ C_{\varepsilon,1} \langle u_{g,i} u_{g,j} \rangle \frac{\partial U_{g,i}}{\partial x_j} + C_{\varepsilon,2} \varepsilon \right] + \sum_p \Pi^\varepsilon_{p \to g}
\end{align*}
\]

Reynolds tensor of gas phase (Boussinesq approximation)

\[
\langle u_{g,i}', u_{g,j}' \rangle = -\nu_g' \left[ \frac{\partial U_{g,i}}{\partial x_j} + \frac{\partial U_{g,j}}{\partial x_i} \right] + \frac{2}{3} \left[ k + \nu_g' \frac{\partial U_{g,m}}{\partial x_m} \right] \delta_{ij}
\]

Model constants

\[
C_{12} = 0.34, C_\mu = 0.09, \sigma_k = 1, \sigma_\varepsilon = 1.3 \]
\[
C_{\varepsilon,1} = 1.44, C_{\varepsilon,2} = 1.92, C_{\varepsilon,3} = 1.2 \]

Influence of particles in fluid turbulence: two-way coupling

\[
\Pi^k_{p \to g} = \frac{\alpha_p \rho_p}{\alpha_g \rho_g} \frac{1}{\tau^p_{gp}} \left[ q_{gp} - 2k + V_{d,i} V_{r,i} \right] \quad \Pi^\varepsilon_{p \to g} = C_{\varepsilon,3} \frac{\varepsilon}{k} \Pi^k_{p \to g}
\]

Closure models for turbulence

Kinetic energy transport equation [1]

\[ \alpha_p \rho_p \left[ \frac{\partial q^2_p}{\partial t} + U_{p,i} \frac{\partial q^2_p}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[ \alpha_p \rho_p \left( K^\text{kin}_p + K^\text{col}_p \right) \frac{\partial q^2_p}{\partial x_j} \right] - \left\langle u^i_{p,j} u^j_{p,i} \right\rangle \frac{\partial U_{p,i}}{\partial x_j} - \frac{\alpha_p \rho_p}{\tau^F_{gp}} \left[ 2q^2_p - q_{gp} \right] + \sum_q \varepsilon_{qp} + \sum_q \chi_{qp} \]

Diffusion of kinetic energy

Production by gradient of the mean of velocity

Interaction with gas phase

Granular stress tensor [2]

\[ \left\langle u^i_{p,j} u^j_{p,i} \right\rangle = -\mu_p \left[ \frac{\partial U_{p,i}}{\partial x_j} + \frac{\partial U_{p,j}}{\partial x_i} - \frac{2}{3} \frac{\partial U_{p,m}}{\partial x_m} \delta_{ij} \right] + \left[ P_p - \lambda_p \frac{\partial U_{p,m}}{\partial x_m} \right] \delta_{ij} \]

Granular viscosity

\[ \mu_p = \alpha_p \rho_p \left( \nu^\text{kin}_p + \nu^\text{col}_p \right) \]

\[ K^\text{kin}_p \quad \text{Kinetic diffusivity} \quad \nu^\text{kin}_p \quad \text{Granular kinetic viscosity} \quad P_p \quad \text{Granular pressure} \]

\[ K^\text{col}_p \quad \text{Collisional diffusivity} \quad \nu^\text{col}_p \quad \text{Granular collisonal viscosity} \quad \lambda_p \quad \text{Bulk viscosity} \]

Dissipation by inelastic collision

Agitation exchange between particles

Closure models for turbulence

Transport equation of correlation fluid particle velocity fluctuation[1]

\[
\alpha_p \rho_p \left[ \frac{\partial q_{sp}}{\partial t} + U_{p,j} \frac{\partial q_{sp}}{\partial x_j} \right] = \frac{\partial}{\partial x_j} \left[ \alpha_p \rho_p \frac{\nu_{sp}'}{\sigma_{qsp}} \frac{\partial q_{sp}}{\partial x_j} \right] - \alpha_p \rho_p \left( \bar{u}_{g,i} \bar{u}_{p,j} \right) \frac{\partial U_{p,i}}{\partial x_j} - \alpha_p \rho_p \left( \bar{u}_{g,j} \bar{u}_{p,i} \right) \frac{\partial U_{g,i}}{\partial x_j} + \Pi_{qsp} - \alpha_p \rho_p \varepsilon_{sp}
\]

Correlation velocity fluctuation gas-particles

\[
\left\langle \bar{u}_{g,i} \bar{u}_{p,j} \right\rangle = -\nu_{sp}' \left[ \frac{\partial U_{g,i}}{\partial x_j} + \frac{\partial U_{p,j}}{\partial x_i} \right] + \frac{1}{3} \left[ q_{sp} + \nu_{sp}' \frac{\partial U_{g,m}}{\partial x_m} + \nu_{sp}' \frac{\partial U_{p,m}}{\partial x_m} \right] \delta_{ij}
\]

Turbulent viscosity

\[
\nu_{sp}' = \frac{1}{3} q_{sp} \tau_{sp}'
\]

Influence of particle on correlation fluid particle velocity fluctuation

\[
\Pi_{qsp} = -\frac{\alpha_p \rho_p}{\tau_{sp}} \left[ \left( 1 + \frac{\alpha_p \rho_p}{\alpha_g \alpha_g} \right) q_{sp} - 2k - 2 \frac{\alpha_p \rho_p}{\alpha_g \alpha_g} q_p^2 \right]
\]

III. Numerical simulation with NEPTUNE_CFD
## Geometry

<table>
<thead>
<tr>
<th>Geometry configuration</th>
<th>Nozzle diameter</th>
<th>0.0142 m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber test dimensions</td>
<td>0.47 m x 0.47 m x 1 m</td>
<td></td>
</tr>
<tr>
<td>Gas properties (air)</td>
<td>Density</td>
<td>1.18 ( kg/m^3 )</td>
</tr>
<tr>
<td></td>
<td>Viscosity</td>
<td>1.85e-05 Pa.s</td>
</tr>
<tr>
<td>Particles properties (glass beads)</td>
<td>Density</td>
<td>2500 ( kg/m^3 )</td>
</tr>
<tr>
<td></td>
<td>Diameters</td>
<td>25 ( \mu m ) and 70 ( \mu m )</td>
</tr>
<tr>
<td>Particle mass loading</td>
<td>Monosized particle</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>Binary mixture</td>
<td>0.5/class</td>
</tr>
</tbody>
</table>
Mesh

3D Structured Mesh

Number of cells: 61,950
Mesh dimension: 0.47 m x 0.47 m x 1 m

\[ \Delta x_{\text{min}} \approx 0.001 m \]
\[ \Delta x_{\text{max}} \approx 0.05 m \]
\[ \Delta y_{\text{min}} \approx 0.001 m \]
\[ \Delta y_{\text{max}} \approx 0.05 m \]
\[ \Delta z_{\text{min}} \approx 0.04 m \]
\[ \Delta z_{\text{max}} \approx 0.12 m \]
Boundary conditions

Mean Velocity:

- Gas phase: interpolated from experimental data
- Particulate phases: interpolated from experimental data

Mean agitation:

\[ k = \frac{1}{2} \left[ u_{g,z}^{\prime 2} + 2u_{g,x}^{\prime 2} \right] \]

k-\( \varepsilon \) model

\[ \varepsilon = C_\mu \frac{k^{1.5}}{l_m} \]

\[ l_m = 0.03D \]

\[ C_\mu = 0.09 \]

\[ q_p - q_{gp}, \text{ model} \]

\[ q_p^2 = \frac{1}{2} \left[ u_{p,z}^{\prime 2} + 2u_{p,x}^{\prime 2} \right] \]

\[ q_{gp} = \frac{1}{2} q_p^2 \quad (\text{Tchen's hypothesis}) \]
Boundary conditions

Particle mass loading for monodisperse case

\[ m = \frac{\int_{A_c} \alpha_p \rho_p U_p \, dA_c}{\int_{A_c} (1 - \alpha_p) \rho_g U_g \, dA_c} \]

Volume fraction of particulate phase

\[ \alpha_p = \frac{m \rho_g U_{g,z}}{m \rho_g U_{g,z} + \rho_p U_{p,z}} \]

For 25 \( \mu \)m particles case and 70 \( \mu \)m particles case

For binary mixture case.

\( \alpha_p \approx 5 \times 10^{-4} \)

\( \alpha_{p,25} \approx 2.5 \times 10^{-4} \quad \alpha_{p,70} \approx 2.5 \times 10^{-4} \)
Numerical results - Single phase flow

Relative pressure field

Velocity field of gas phase

Radial profiles

X/D=1
X/D=3
X/D=5
X/D=10
X/D=15

Axial profile

D: nozzle diameter

Physical time: 2s. Established regime
Numerical results - Single phase flow

Axial velocity profiles

Radial velocity profiles at Inlet

Radial profiles of gas velocity Ugz

Ugz: axial component of gas velocity
Numerical results - Two-phase flow with 25 μm particles

Relative pressure field

Volume fraction field of particulate phase

Velocity field of gas phase

Velocity field of particulate phase

Axial profile

D: nozzle diameter

Physical time: 2s. Established regime
Numerical results- Two-phase flow with 25 μm particles

- $\alpha_p$: volume fraction of particulate phase

$U_{gz}$: axial component of gas velocity

$U_{pz}$: axial component of particulate velocity

$U_{px}$: radial component of particulate velocity

$\uparrow$ Turbophoresis phenomenon
Numerical results - Two-phase flow with 70 μm particles

Relative pressure field
-3.711e-01
-3.623e+00
-6.875e+00
-1.013e+01
-1.338e+01

Volume fraction field of particulate phase
0.000e+00
1.328e-04
2.657e-04
3.985e-04
5.313e-04

Velocity field of gas phase
1.082e+01
3.014e+00
8.114e+00
1.798e+00
5.411e+00

Velocity field of particulate phase
2.708e+00
4.356e-03
9.839e+00
7.404e+00
4.988e+00

Physical time: 2s. Established regime
Numerical results - Two-phase flow with 70 μm particles

\( \alpha_p \)  
volume fraction of particulate phase

\( U_{gz} \): axial component of gas velocity

\( U_{pz} \): axial component of particulate velocity

\( U_{px} \): radial component of particulate velocity
Numerical results - Two-phase flow with binary mixture

Relative pressure field

Volume fraction field of 25 μm particulate phase

Volume fraction field of 70 μm particulate phase

Physical time: 2s. Established regime
Numerical results - Two-phase flow with binary mixture

Velocity field of 25 μm particulate phase

Velocity field of 70 μm particulate phase

Physical time: 2s. Established regime

Radial profiles

Axial profile

D: nozzle diameter

X/D=5
X/D=10
X/D=15
Numerical results - Two-phase flow with binary mixture

$\alpha_{p2}$ volume fraction of 25 $\mu$m particulate phase

$\alpha_{p3}$ volume fraction of 70 $\mu$m particulate phase
Numerical results - Two-phase flow with binary mixture

Axial velocity profiles

Radial velocity profiles at Inlet

Upz: axial component of gas velocity

Upz2: axial component of particulate velocity of 25 μm particle

Upx2: radial component of particulate velocity of 25 μm particle

Upz3: axial component of particulate velocity of 70 μm particle

Upx3: radial component of particulate velocity of 70 μm particle
IV. Conclusions and perspectives

Conclusions

• Good agreement between numerical simulation and experimental results is obtained
• Some differences are mainly observed for 70 μm particle for monodisperse and binary mixture cases.

Outlook

• The numerical simulation with Code_Saturne is on going.
• The modelling of brownian motion and agglomeration for nanoparticle will be implemented to numerical tools Neptune_CFD and/or Code_Saturne.
Thank you for your attention!