Large Eddy Simulation of turbulent circular jet using OpenFOAM

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2019
Siemens technology (based on chemical vapor deposition) is widely used for polysilicon production.

Silicon containing gas mixture is supplied by turbulent jet.

Heat exchange and mass transport are determined by turbulent fluctuations.

Numerical modeling is required to improve reactor characteristics.

**Motivation**

Polysilicon deposition reactor
The experimental set-up and computational domain

\[ Re = D_j U_j / \nu = 21000 \]

\[ m = U_e / U_j = 0.075 \]


\[ U^n = (1-\alpha)U^{n-1} + \alpha (U_j + r \cdot s \cdot C \cdot U_j) \]

\[ \alpha = 0.25, \ s = 0.05 \]
1. Models
   - LES WALE model
   - Implicit LES (ILES) approach
2. Codes
   - OpenFOAM (PIMPLE solver from incompressible group)
   - SINF/Flag-S (original version of the implicit fractional-step method to advance in physical time)
3. Numerical schemes: LUST, QUICK, Linear Upwind, Linear
4. The approximation of the time derivative was carried out with the second-order scheme “backward”
1. Original mesh: 1.3 mln cells
   Typical cell size ~ 0.004 m, 22 cells/$D_j$
2. Fine mesh: 11 mln cells
   Typical cell size ~ 0.002 m, 40 cells/$D_j$
3. Coarse mesh: 0.2 mln cells
   Typical cell size ~ 0.08 m, 12 cells/$D_j$
Instantaneous and averaged distributions of velocity magnitude
Instantaneous and averaged distributions of velocity magnitude
Instantaneous and averaged distributions of velocity magnitude
Comparison with the experimental data

- Experiment Djeridane et al.
- Experiment Abramovich $U_e/U_j = 0$
- Experiment Abramovich $U_e/U_j = 0.114$
- Experiment Shahriar et al., 2011

- OpenFOAM WALE
- OpenFOAM ILES
- SINF/Flag-S ILES
- Analytical solution
- P. Wang et al.*

* Ping Wang, Jochen Fröhlich, Vittorio Michelassi, Wolfgang Rodi
“Large-eddy simulation of variable-density turbulent axisymmetric jets”,

The distribution of longitudinal component of the averaged velocity along the jet axis
Comparison with the experimental data

The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis

- Experiment Djeridane et al.
- OpenFOAM WALE
- OpenFOAM ILES
- SINF/Flag-S ILES
- P. Wang et al.

The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis
The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis.

\[ \Delta \tau = \Delta t \frac{U_j}{D_j} = 0.11 \]

The distribution of the averaged longitudinal component of the averaged velocity along the jet axis.
The distribution of longitudinal component of the averaged velocity along the jet axis

$\Delta \tau = \Delta t U_j / D_j = 0.11$

Fine mesh

- Exp. Djeridane et al.
  - $\Delta \tau = 0.46$, $CFL_{x/D_j=20} = 1.6$
  - $\Delta \tau = 0.23$, $CFL_{x/D_j=20} = 0.8$
  - $\Delta \tau = 0.11$, $CFL_{x/D_j=20} = 0.4$
  - $\Delta \tau = 0.06$, $CFL_{x/D_j=20} = 0.2$
The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis

The distribution of the RMS-fluctuation of longitudinal velocity component along the radius in the section $x/D_j = 20$

- Exp. Djeridane et al.
  - $\Delta \tau = 0.46$, $CFL_{x/D_j} = 20 = 1.6$
  - $\Delta \tau = 0.23$, $CFL_{x/D_j} = 20 = 0.8$
  - $\Delta \tau = 0.11$, $CFL_{x/D_j} = 20 = 0.4$
  - $\Delta \tau = 0.06$, $CFL_{x/D_j} = 20 = 0.2$
Courant number sensitivity

- Experiment Djeridane et al.

- Coarse mesh $\Delta \tau = 0.92$, $CFL_{x/D_j = 20} = 1.2$
- Coarse mesh $\Delta \tau = 0.46$, $CFL_{x/D_j = 20} = 0.5$
- Original mesh $\Delta \tau = 0.46$, $CFL_{x/D_j = 20} = 0.8$
- Original mesh $\Delta \tau = 0.23$, $CFL_{x/D_j = 20} = 0.4$
- Fine mesh $\Delta \tau = 0.46$, $CFL_{x/D_j = 20} = 1.6$
- Fine mesh $\Delta \tau = 0.23$, $CFL_{x/D_j = 20} = 0.8$

$CFL_{max} \sim 5 \div 10$

The distribution of the RMS-fluctuation of longitudinal velocity component along the radius in the section $x/D_j = 20$
Influence of numerical scheme

The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis

- Experiment
- LUST
- QUICK
- Linear Upwind
- Linear

The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis
The distribution of the RMS-fluctuation of longitudinal velocity component along the jet axis

\[ U^n = (1-\alpha)U^{n-1} + \alpha (U_j + r \cdot s \cdot C \cdot U_j) \]

- Experiment
  - $\alpha = 0.25$, $s = 0.1$
  - $\alpha = 0.25$, $s = 0.025$
  - $\alpha = 0.25$, $s = 0.05$
  - $\alpha = 0.1$, $s = 0.05$
  - $\alpha = 0.5$, $s = 0.05$
For accurate modeling of averaged characteristics it is recommended to use original \((22 \text{ cells}/D_j)\) or coarse \((12 \text{ cells}/D_j)\) mesh.

For accurate modeling of fluctuation characteristics it is recommended to use fine \((40 \text{ cells}/D_j)\) mesh.

It is possible to use time step corresponding to 
\[CFL_{max} \sim 10,\] but it is desirable to achieve 
\[CFL < 1\] at the main jet region.

Results obtained by LES WALE and ILES are almost similar.

Influence of considered numerical schemes on the solution is quite small, except linear scheme, which gives non-physical pulsations.

The LUST or QUICK scheme is recommended to use in LES.

The small solution sensitivity to the synthetic generator parameters was also observed.
The longitudinal component of the RMS-fluctuation velocity field for solutions obtained by OpenFOAM (a) and SINF/Flag-s (b)