Participation of EDF to the OECD/NEA CFD-UQ benchmark: GEMIX

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Table of content

- Test case description
- CFD setup
- Results
- Conclusion
Test case description
OECD/NEA CFD-UQ benchmark

GEMIX: GEnering MIxing eXperiment exploited at PSI in Switzerland.
OECD/NEA CFD-UQ benchmark

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Proposal to participate sent to:

- Nuclear Regulatory Commission (NRC - USA)
- Instituto Ingeniería Energética (IIE - Spain)
- Consejo de Seguridad Nuclear (CSN - Spain)
- Électricité De France (EDF - France)
- Areva (France)
- Gesellschaft für Anlagen und Reaktorsicherheit (GRS - Germany)
- Nuclear Regulation Authority (NSR - Japan)
- National Research Nuclear University (Russia)
- Institut “Jozef Stefan” (IJS - Slovenia)
- Paul Scherrer Institute (PSI - Switzerland)
- Nuclear Research and Consultancy Group (NRG - Holland)
- National Centre for Nuclear Research (NCBJ - Poland)
- National Skills Academy for Nuclear (NSAN - GB)
- Energia e lo Sviluppo economico sostenibile (ENEA - Italia)
- Ansys (USA)
- ...

4/37  
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OECD/NEA CFD-UQ benchmark

Specifications of the test case:
“The main objective of this exercise is to compare and evaluate different UQ methodologies, currently used to assess the reliability of CFD simulations in the presence of several sources of uncertainties.”

Also, according to these specifications, no guidance on:
- the uncertain parameters to take into account,
- the methodology to compute uncertainty bands,
- the numerical schemes, turbulence models, computational mesh.

A $2 \times 2$ matrix of experiments has been performed. For one experiment, the participants have no measurement results.
Preliminary physical analysis

Highlights:

- co-current flows of equal velocities;
- difference in density between 0 and +1% for lower leg;
- grids at the inlets at $x = -520 \text{ mm}$, $x = -300 \text{ mm}$ and $x = -80 \text{ mm}$;
- measurement of $U$, $R_{11}$, $R_{22}$, $R_{33}$ at $x = -50 \text{ mm}$.

At the junction of the inlets, the flows are “between” fully developed and decaying isotropic turbulence \(^a\). After the junction, the boundary layers at $y = 0$ decay and the flow evolves towards a turbulent square-section channel flow.

\(^a\)Neglecting the influence of downstream towards upstream
## Preliminary PIRT

From *engineer judgement* one infers:

<table>
<thead>
<tr>
<th>Physical phenomena</th>
<th>Non dim. numbers</th>
<th>Parameters</th>
<th>Influence</th>
<th>Level of knowledge</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary layer</td>
<td>$Re$</td>
<td>Velocity, TKE</td>
<td>High</td>
<td>Medium</td>
<td>Input data from measures</td>
</tr>
<tr>
<td>Mixing</td>
<td>$Re$, $Fr$</td>
<td>Velocity, TKE, $\Delta \rho$</td>
<td>High</td>
<td>Medium</td>
<td>Goal of the simulations</td>
</tr>
<tr>
<td>Recirculation</td>
<td>$Re$</td>
<td>Velocity, TKE</td>
<td>Low</td>
<td>Medium</td>
<td>Probably not happening</td>
</tr>
<tr>
<td>Stratification</td>
<td>$Re$, $Fr$</td>
<td>Velocity, TKE, $\Delta \rho$</td>
<td>Low</td>
<td>Medium</td>
<td>Froude too high</td>
</tr>
</tbody>
</table>
Matrix of experiments

$\Delta \rho/\rho$

$Re$

(11) (21)

(12) (22)

$Re_1 = 30000$

$Re_2 = 50000$

$(\Delta \rho/\rho)_1 = 0$ ($Fr_1 = +\infty$)

$(\Delta \rho/\rho)_2 = 1\%$ ($Fr_2$, $Re = 30000 = 8.5$, $Fr_2$, $Re = 50000 = 14.3$)

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Matrix of experiments

Non dimensional numbers in the mixing section

\[ Re_1 = 30000 \]
\[ Re_2 = 50000 \]
\[ (\Delta \rho / \rho)_1 = 0 \quad (Fr_1 = +\infty) \]
\[ (\Delta \rho / \rho)_2 = 1\% \quad (Fr_2, Re=30000 = 8.5, \quad Fr_2, Re=50000 = 14.3) \]
CFD setup (Code_Saturne 4.2)
Mesh sensitivity

Domain divided by 2 by symetry (plane $z = 0$).

3 “low-Reynolds” grids made with SALOME with a uniform refinement ratio of 1.5.
- 193 920 cells,
- 652 320 cells,
- 2 196 720 cells.
Mesh sensitivity

Domain divided by 2 by symmetry (plane $z = 0$).

3 “low-Reynolds” grids made with SALOME with a uniform refinement ratio of 1.5.

- 193,920 cells,
- 652,320 cells,
- 2,196,720 cells.

The middle size one has been selected after post-processing.
Interpolation of BCs

In `cs_user_boundary_conditions.f90`

- Velocities: **linear**
Interpolation of BCs

- Reynolds stresses: **cubic splines** \( \left( \frac{\partial R_{ii}}{\partial y} \big|_{y=0} = 0 \right) \)

- Non measured parameters are given a **Neumann condition**.
Uncertain parameters

Inlet conditions given with uncertainties

- for sheets of $U$, $V$ and $W$ a 95% percentile,
- for sheets of $R_{11}$, $R_{22}$ and $R_{33}$ a lower and a upper sheet,
- for $\Delta \rho$ a lower and upper value of $\pm 0.01 \text{ kg/m}^3$.

---

\( ^a \text{Simple Gradient Diffusion Hypothesis} \)
\( ^b \text{Generalized Gradient Diffusion Hypothesis} \)
**Uncertain parameters**

**Inlet conditions given with uncertainties**

- for sheets of $U$, $V$ and $W$ a 95% percentile,
- for sheets of $R_{11}$, $R_{22}$ and $R_{33}$ a lower and an upper sheet,
- for $\Delta \rho$ a lower and upper value of $\pm 0.01 \text{ kg/m}^3$.

From these data, it was decided to consider:

- an uncertain sheet of axial velocity, $U = U_{\text{mean}} + X_U \frac{U_{95}}{2}$ with $X_U \sim N(0, 1)$
- an uncertain sheet of Reynolds stresses, $R_{ii} = R_{ii,\text{min}} + X_k (R_{ii,\text{max}} - R_{ii,\text{min}})$ with $X_k \sim U(0, 1)$

Plus, since prediction of turbulence is the key to expect correct results,

- 2 different turbulence models: the $k - \omega$ with SGDH$^a$ and the EB-RSM with GGDH$^b$.

---

$^a$Simple Gradient Diffusion Hypothesis  
$^b$Generalized Gradient Diffusion Hypothesis
Design Of Experiment (D.O.E)

with OpenTURNS:

```python
import openturns as ot
ot.RandomGenerator.SetSeed(0)
nDist = ot.Normal(0., 1.)
uDist1 = ot.Uniform(0., 1.)
uDist2 = ot.Uniform(-1., 1.)
aColl = [nDist, uDist1, uDist2]
cDist = ot.ComposedDistribution(aColl)
experiment = ot.LHSExperiment(cDist, 6)
print(experiment.generate())
```

Nota Bene: 6 calculations do not ensure convergence of statistics but the effort to put in propagation of uncertainties has to be balanced by the dispersion the uncertain parameters lead to and by the level of knowledge of these parameters. In dimension 3 with 6 realizations, it was possible to use an optimal D.O.E (this one seems far from optimality).
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<table>
<thead>
<tr>
<th>X&lt;sub&gt;k&lt;/sub&gt;</th>
<th>EB-RSM</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.00</td>
<td>-0.97</td>
</tr>
<tr>
<td>0.17</td>
<td>-0.43</td>
</tr>
<tr>
<td>0.33</td>
<td>0.00</td>
</tr>
<tr>
<td>0.50</td>
<td>0.43</td>
</tr>
<tr>
<td>0.67</td>
<td>0.97</td>
</tr>
<tr>
<td>0.83</td>
<td>0.43</td>
</tr>
<tr>
<td>1.00</td>
<td></td>
</tr>
</tbody>
</table>

Nota Bene:

- **6 calculations do not ensure convergence of statistics** but the effort to put in propagation of uncertainties has to be balanced by the dispersion the uncertain parameters lead to and by the level of knowledge of these parameters.

- In dimension 3 with 6 realizations, it was possible to use an **optimal D.O.E** (this one seems far from optimality).
Results
Validation

For 3 experiments, measurements of $U$ and $C$ (and $k$ not presented here) at $x = 50 \text{ mm}$, $x = 150 \text{ mm}$, $x = 250 \text{ mm}$, $x = 350 \text{ mm}$ and $x = 450 \text{ mm}$ are available. We compare the uncertainty bands (95% percentile) of the measures with the results of the propagation of uncertainties.
Sensitivity analysis

The sensitivity analysis is performed with a Polynomial Chaos Expansion confronted to the over-learning phenomenon with a Leave-One-Out technique. Logically, the 6 calculations do not allow to capture more than first order effects and the response surface respects:

\[ y = a_y,0 + a_y,U X_U + a_y,k X_k + a_y,mod X_{mod} \]
Extrapolation of errors outside the domain of validation

Hypothesis: linear evolution of errors,

\[ e_{xy} = a_0 + a_1 x + a_2 y \implies e_{22} = e_{12} + e_{21} - e_{11}. \] (1)
Extrapolation of errors outside the domain of validation

Hypothesis: linear evolution of errors,

\[ e_{xy} = a_0 + a_1 x + a_2 y \implies e_{22} = e_{12} + e_{21} - e_{11}. \] (1)

We introduce relative errors on mean value and standard deviation:

\[
\begin{align*}
    e_\mu &= \frac{\mu^M}{\mu^C} \\
    e_\sigma &= \frac{\sigma^M}{\sigma^C},
\end{align*}
\]

with \( ^M \) for measured results and \( ^C \) for results of CFD.
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Hypothesis: **linear evolution of errors**, 

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(1)

We introduce **relative errors** on mean value and standard deviation:

\[ e_\mu = \frac{\mu^M}{\mu^C}, \]

\[ e_\sigma = \frac{\sigma^M}{\sigma^C}, \]

with \( M \) for measured results and \( C \) for results of CFD.

Using these errors on mean value and standard deviation extrapolated with equation (1), it is possible to **calculate what measurement results would be** in case (22),

\[ y_i^{\text{extrap}} = (y_i^C - \mu^C) e_{\sigma, 22} + \mu^C e_{\mu, 22} \]  

(2)
Conclusion
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- GEMIX test case potentially interesting for different nuclear applications: boron dilution, PTS\(^a\), SLB\(^b\), ....
- The uncertainties considered on input parameters do not make calculations and measurements overlap.
- The most influential parameter is the turbulence model with the EB-RSM + GGDH allowing to get results closer from measurements.
- Under certain circumstances and with sufficient care in exploitation of results it seems possible to use limited numbers of calculations.

\(^a\)Pressurized Thermal Shock
\(^b\)Steam Line Break
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\textsuperscript{a}Pressurized Thermal Shock
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Thank you for your attention
Appendix
\[ y \ (\text{mm}) \]

\[ 10^3 \times k \ (m^2/s^2) \]

coarse
med
fine