Automatic workflow for SCR-DeNOx optimization

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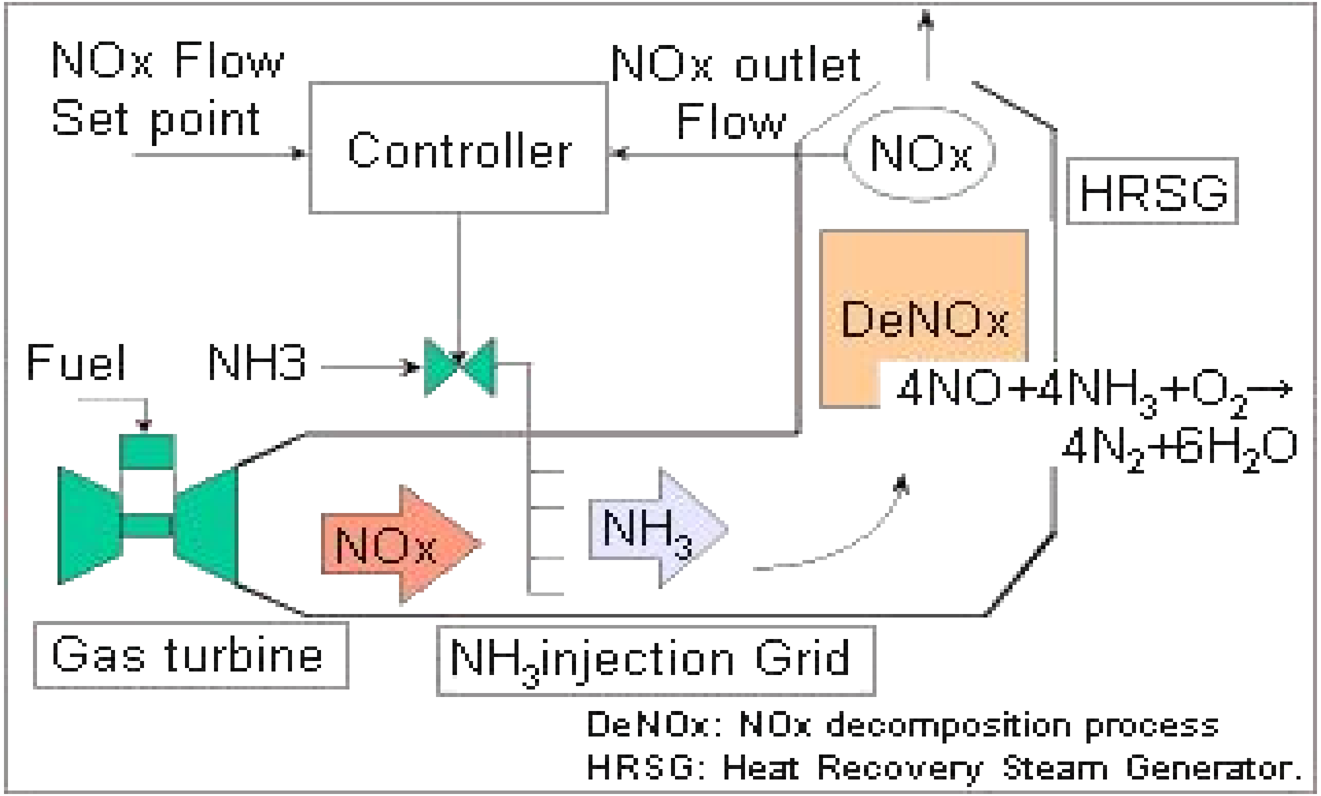
Contents

Introduction

- NOx cause airway problems and it’s necessary to control NOx emissions.
- Control technologies for NOx emissions
  - Primary control technologies: low-emission burners, 50% efficiency
  - Secondary control technologies
    - Non-catalytic selective reduction, high temperatures (1000°C) and 65% efficiency
    - Selective catalytic reduction (SCR-DeNOx), low temperatures (350°C) and 95% efficiency

	SCR	SNCR	HYBRID
Efficiency	Up to 95%	Up to 65%	Up to 90%
Reactant	Ammonia	Ammonia	Ammonia
Investment cost	High	Low	Intermediate

Introduction



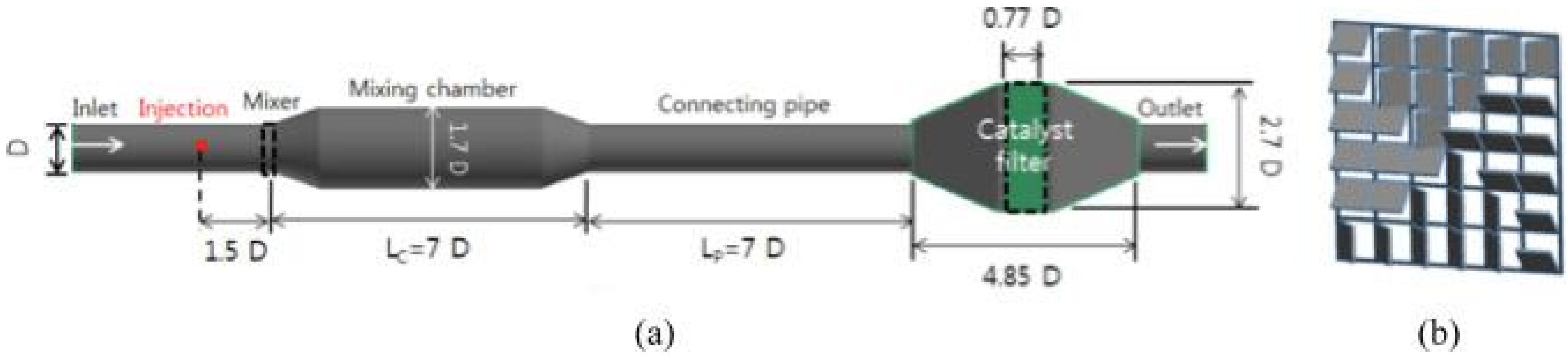
SCR-DeNOx plant scheme

Introduction

SCR-DeNOx plants apply to many different problems, using always the same operating principles:

- Diesel engines
- Gas turbines
- Coal-fired power plants

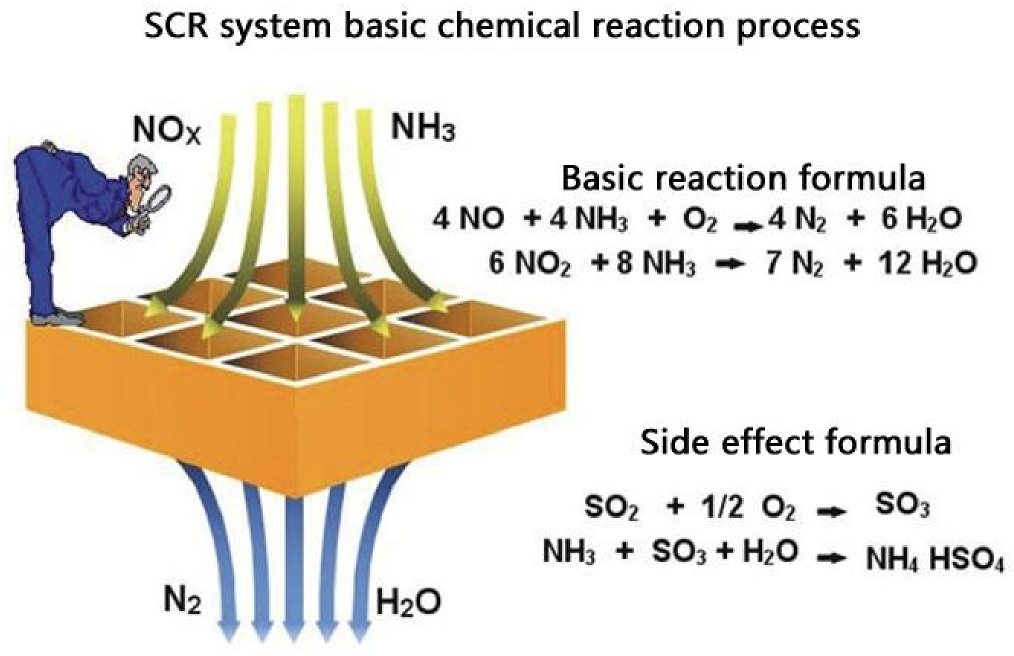
Of particular interest, is the application of SCR-DeNOx systems applied to cogeneration plants, downstream of bio-diesel engines.



Automotive application

Catalyst

SCR-DeNOx plants use a catalyst where chemical reaction to reduce NOx presence take place:



Scheme of a DeNOx catalyst

Non-uniform velocity field at catalyst entrance can cause failures corresponding to velocity peaks

Automated Workflow

Usually, optimised configuration is chosen through designer experience and a trial & error method. Geometry is modified manually and CFD tests are executed on few configurations (2-3 geometries a day).

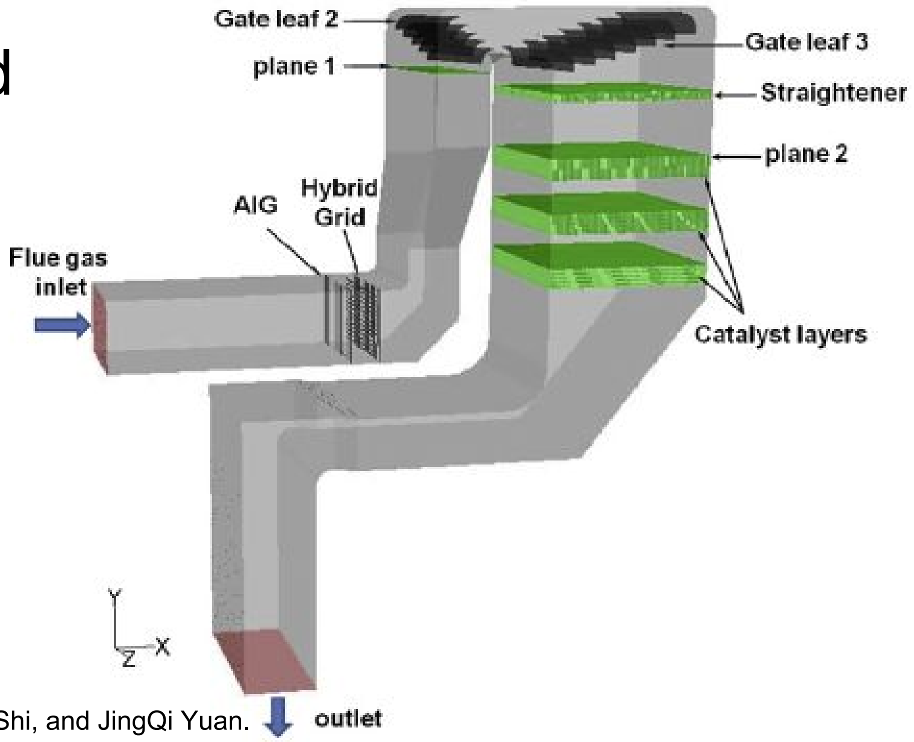
The goal of my work is to implement an automatic workflow:

- Automated geometry changes
- Application of an optimization algorithm

The automatic workflow gives the possibility many more configuration and have a better idea about the effects of turning vanes rotation.

Standard configuration of SCR-DeNOx plants

- Ammonia injection grid (AIG)
- Hybrid grid
- Turning Vanes
- Rectifier
- Catalyst

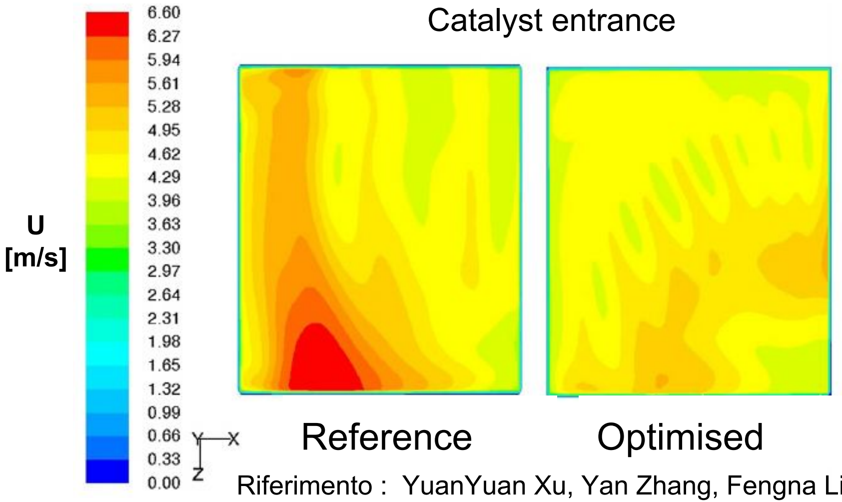


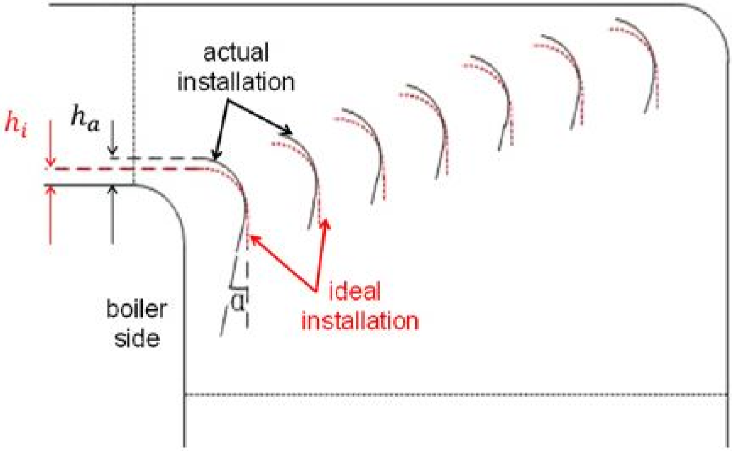
Reference : YuanYuan Xu, Yan Zhang, Fengna Liu, Weifeng Shi, and JingQi Yuan. CFD analysis on the catalyst layer breakage failure of an scr-denox system for a 350 mw coal-fired power plant. Computers and Chemical Engeneering, 69:119–127, 2014

Design of an SCR-DeNOx plant

- First objective: uniform distribution of velocity field at catalyst entrance
- To reach the goal it is possible to change the angle of attack of the turning vanes

These two informations can be considered as the most important references for the automated optimization process



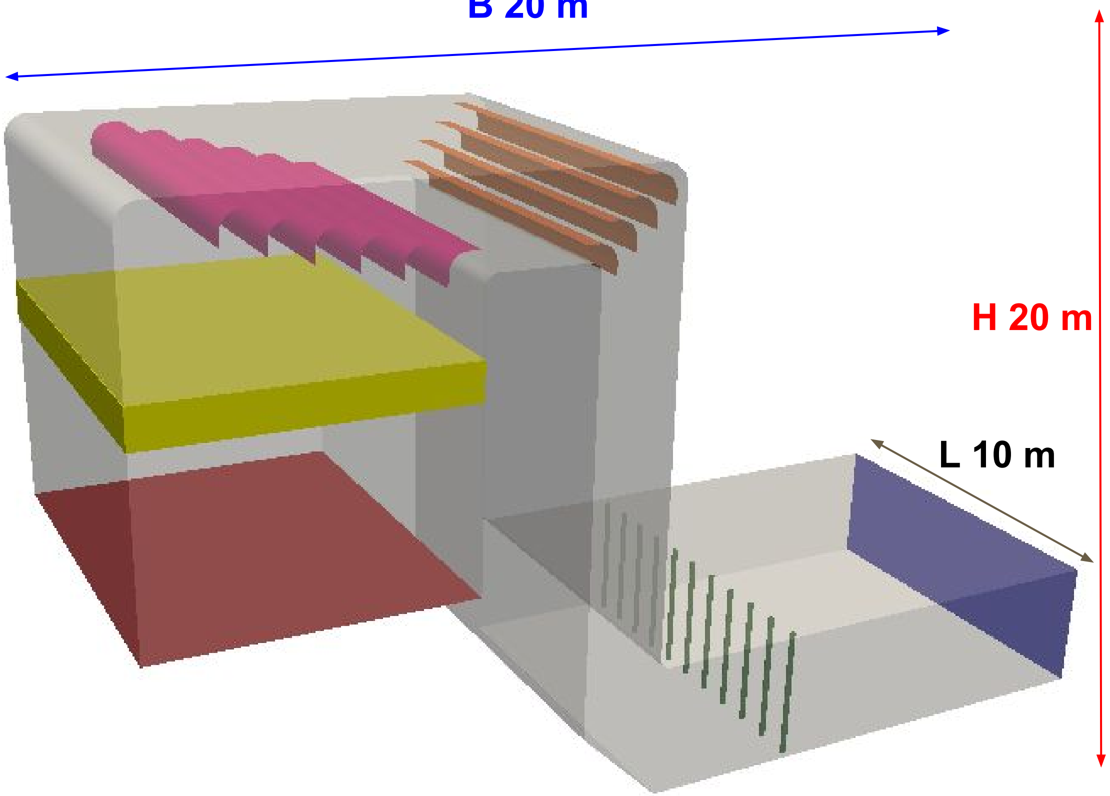


Riferimento : YuanYuan Xu, Yan Zhang, Fengna Liu, Weifeng Shi, and JingQi Yuan.
CFD analysis on the catalyst layer breakage failure of an scr-denox system for a 350 mw coal-fired power plant.
Computers and Chemical Engeneering, 69:119–127, 2014

Selected Geometry

Elements:

- Inlet (blue)
- Ammonia injection grid
- Turning Vanes
- Catalyst
- Outlet (red)



Modelling

Problem	Time	Chemical Reactions	Heat exchange	Turbulence	Catalyst
Real	x	x	x	x	x
Modelled	x	x	x	x	x

- The real problem is multi-physical
- In literature, the problem modelling is:
  - Stationary and incompressible
  - No chemical reactions
  - No heat exchange
  - Turbulence

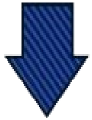
- My CFD setup is:
  - SIMPLE
  - Boundary conditions: inlet 4 m/s with uniform profile, outlet zero pressure
  - Turbulence model: k-omega SST with standard wall functions
  - Catalyst modelled as porous mean

Optimization

In this problem, we have only one objective function with no constraints. In this case, Dakota user's manual suggests to use the conjugate gradient method.

Unconstrained Optimization

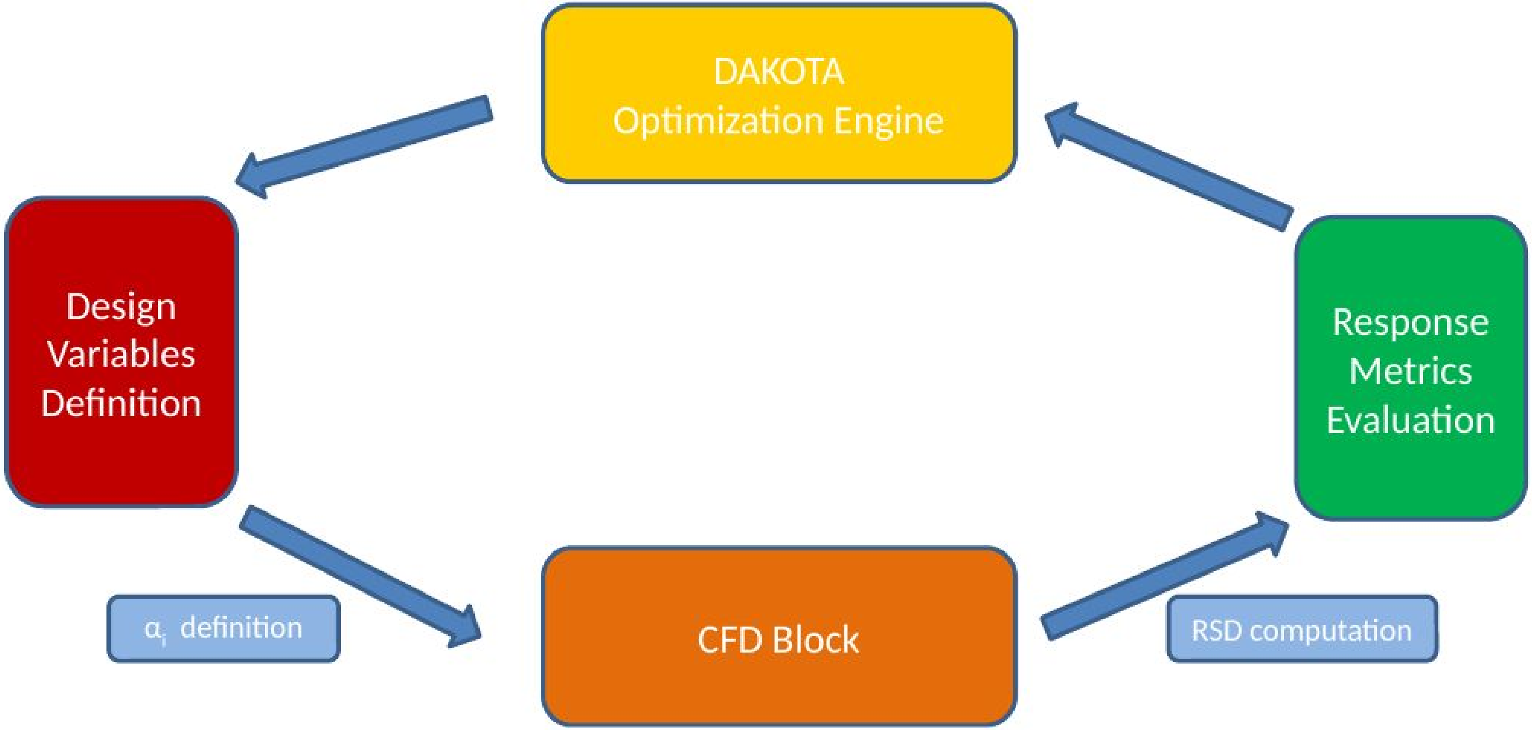
- Parameters: angles of attack of the turning vanes
- Obj function: RSD of the velocity field at catalyst entrance



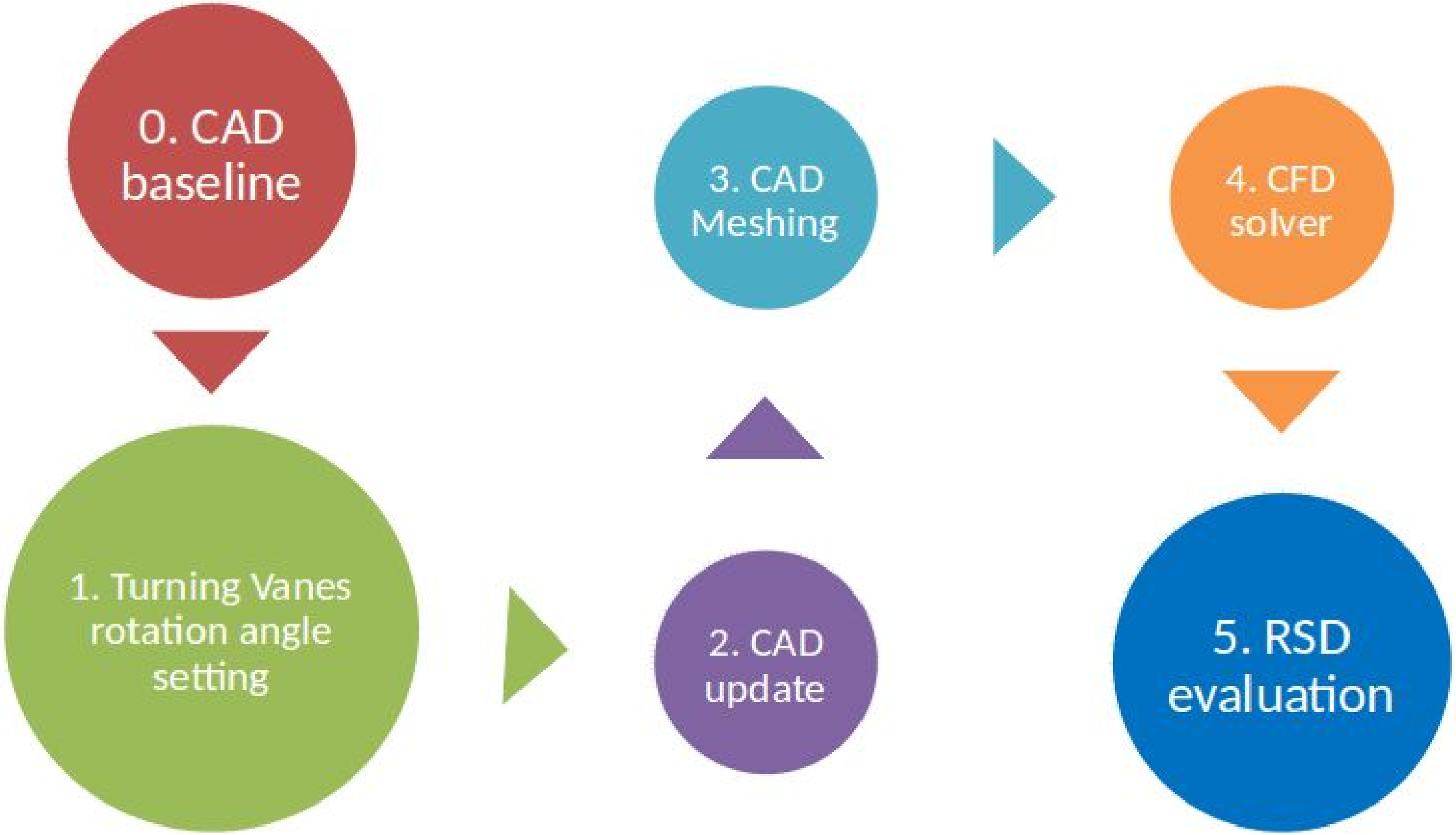
Conjugate gradient method

Optimization

Optimization is managed by Dakota



CFD Block


0. CAD baseline
1. Turning Vanes rotation angle setting
2. CAD update
3. CAD Meshing
4. CFD solver
5. RSD evaluation

Turning vanes rotation

The CFD Block gets the rotation angles as an input from the optimisation engines:

- Single turning vanes are defined in different **.stl* files
- Turning vanes rotation accomplished through a python script
- Every other CAD parameter remains unchanged

CFD Block output: RSD computation

- RSD computation is performed through a Python Script
- Velocity field values are defined in an output file (VTK format) generated by OpenFoam
- RSD formula:

$$\frac{\sqrt{\sum_{i=1}^{n}(u_i - U_{avg})^2}}{(n-1)^{0.5} * U_{avg}}$$

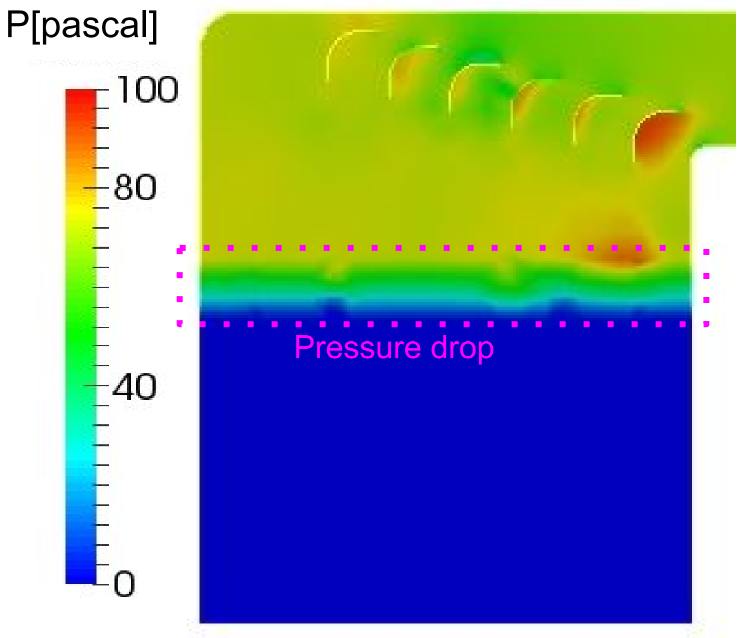
Where:

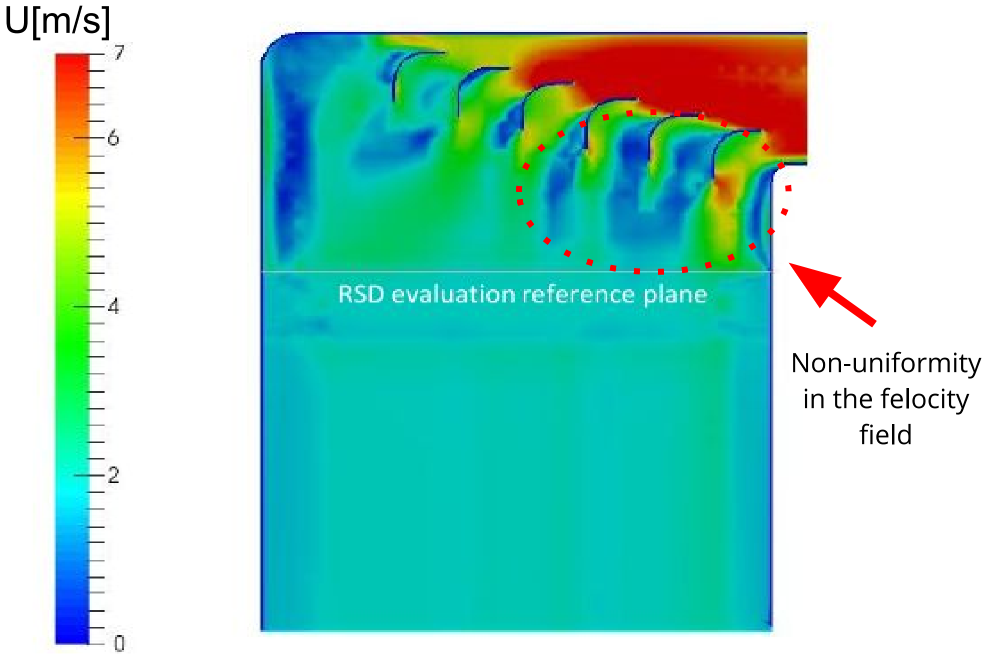
n is the number of mesh cells, Uavg is the mean velocity and u_i is the velocity value on the i-th cell.

The RSD value is used as input for the optimisation engine

Results: reference geometry

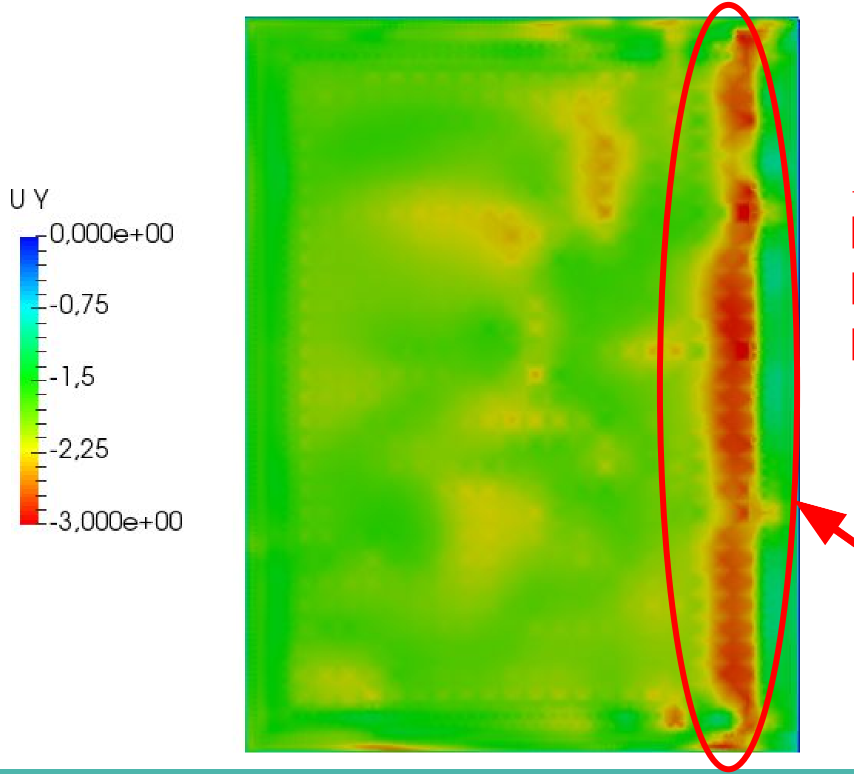
Starting from reference configuration, we obtain these pressure (left figure) and velocity (right figure) fields. It’s important to notice the pressure drop corresponding to the catalyst and the non-uniformity of the velocity field in the last corner.





Results: reference geometry

For the reference configuration, we can see the velocity field at catalyst entrance.

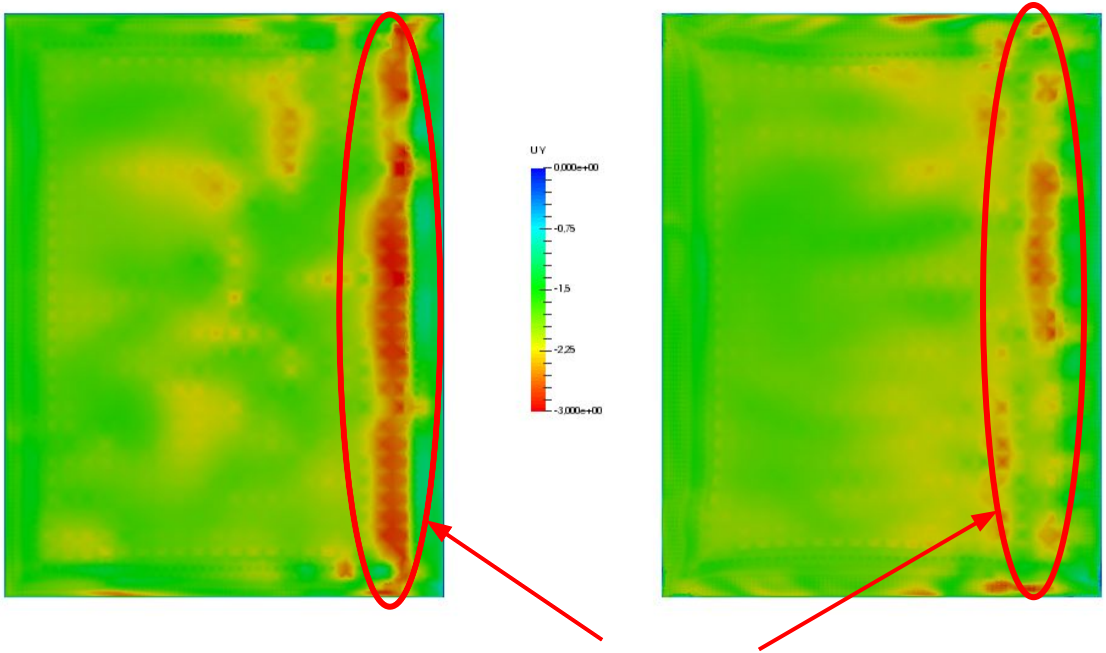


RSD = 54%

Great non-uniformity in the velocity field.
Velocity peaks can cause catalyst failure

Results: optimised configuration

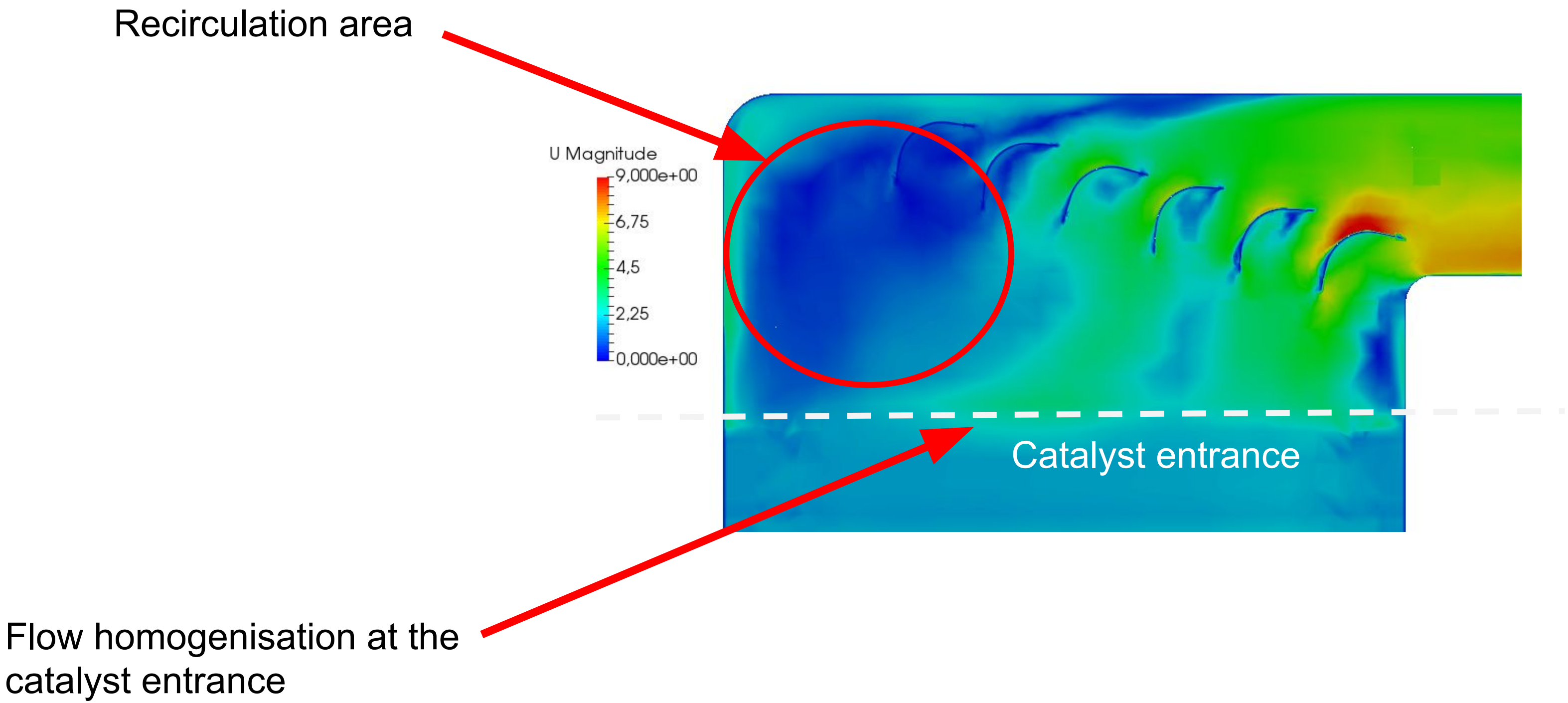
Rotating turning vanes in corner 3, we can notice a great reduction of RSD value, from 54% to 42%



Velocity peak is considerably reduced

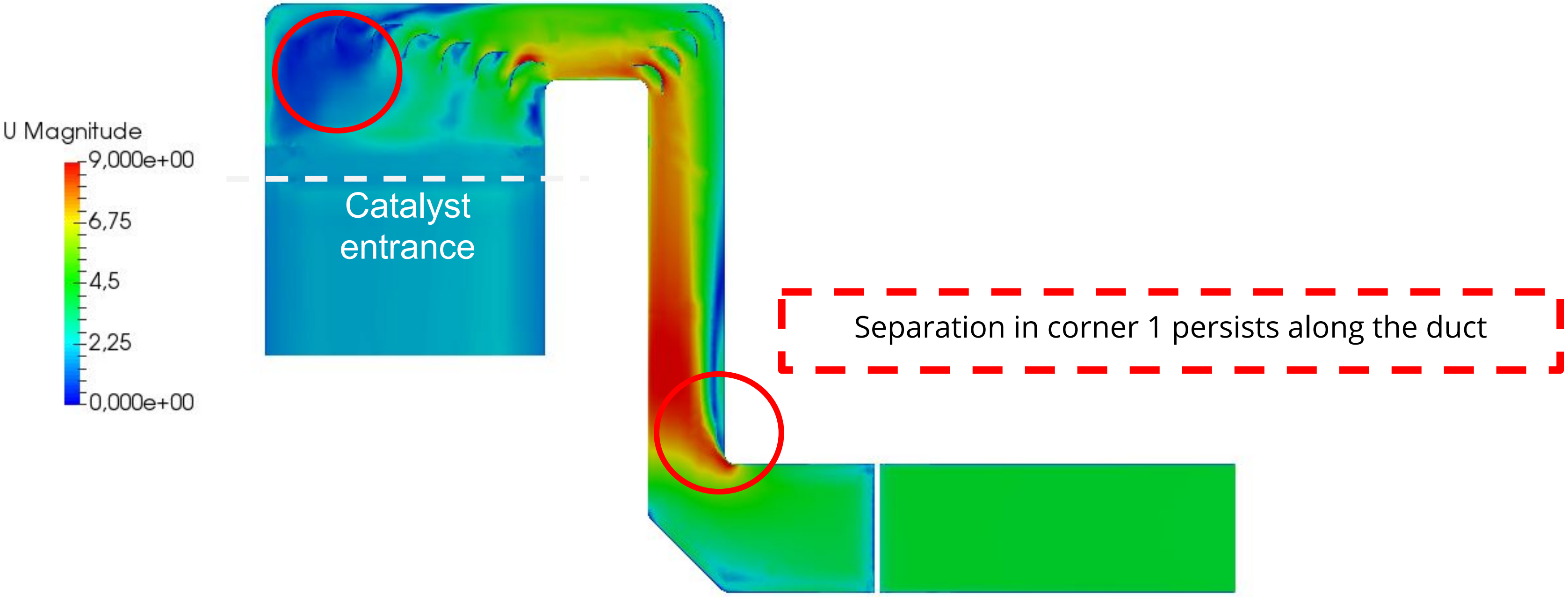
Results: optimised geometry

In corner 3, it is possible to notice a big recirculation area



Results: optimised geometry

Recirculation area in corner 3 is probably due to a separation in corner 1



Conclusions

1. Automated workflow works good: 12% RSD value reduction
2. Non uniformity in corner 3 probably due to separation in corner 1
3. Open-source softwares and HPC platform: 60 configurations tested in 12 hours

Thanks to open-source softwares and HPC platforms, it was possible to evaluate about 60 different configurations in only 12 hours:

- Using 64 cores for a single CFD run
- Total optimization loop using about 800 core-hours

Perspectives

The workflow has been proven to be effective on a real life test case, nevertheless there are many possible improvements:

- Improve the modelling of the physics to be included (ammonia injection, particulates deposition and evaporation; thermal properties)
- Include turning vanes also at corner 1
- Improve RSD calculation including grid topology information at wall
- Include an objective function on the orientation of the flow acting on the porous media (catalyst)

Contacts

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