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LES and DNS Simulations of Imperfect Mixing for Double-Tee Junctions

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Abstract

One critical enhancement needed to model contaminant intrusion in water distribution network is to take into account imperfect mixing at junctions. This paper completes previous work by conducting LES and DNS CFD calculation and laboratory experiments. Statistics were compiled on large-size networks in France and Germany to serve to design a test rig and supply CFD cases for the numerical simulation. The main influencing factors were identified to be: the inter-Tee distance and three of the Reynolds numbers of the inlets/outlets. A lookup table and interpolation methods are used to model inside a one-dimensional model. This is implemented in the transport module of Porteau software.

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Keywords: Transport model; CFD; LES; DNS; imperfect mixing; double-Tee junction.

1. Introduction

The work presented in this paper is part of the French-German collaborative research project SMaRT-Online^{WDN} that is funded by the French National Research Agency (ANR) and the German Federal Ministry of Education and Research (BMBF). The aim of the SMaRT-Online^{WDN} project is to develop an online security management toolkit for water distribution networks (WDN's). How to manage the data to produce alarms, to improve the water quality and water quantity and to secure the network are the largest questions needed to be answered. One critical enhancement needed is to take into account imperfect mixing at junctions.

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In today's software, mixing at junctions is usually made by perfect mixing. Recently, different studies have been carried out to determine a law for imperfect mixing concerning cross and double-Tee junctions. Sandia [1] and the University of Arizona [2] have developed models for cross-junctions and yield first results for double-tee junctions, which gave rise to EPANET-BAM and AZRED implementations. BAM was developed for mixing at cross-junctions, by using a parameter "s" (determined through calibration) to balance between perfect mixing and an ideal bulk-advection model. Cross and double-T junctions AZRED model is based on a lookup table built on laboratory experimental values, and uses interpolation/extrapolation to predict mixing sharing. Mathias Braun *et al.* [3] presented a 2D CFD model at the CCWI 2013, which gives good comparisons with the AZRED model. The 2D CFD simulation was made using COMSOL. They chose to focus on Double-Tee junctions only as crosses have been well covered by BAM and AZRED. This study was performed with 3D simulations: Direct numerical simulation (DNS) for laminar regimes and LES for turbulent regimes and were made with Ansys Fluent [4] and Code Saturne [5] software).

In the first part, the methods and material to do the simulations are described. The second part gives the design of the experiment as well as a method to determine new points of simulation using Voronoï tessellation. Finally, some results of the simulations and methods are given and commented.

2. Methods and material

2.1. Case studies

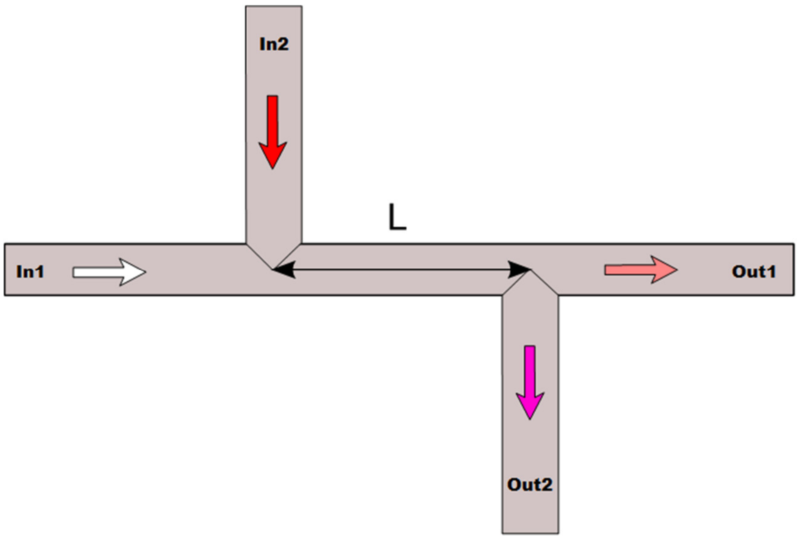

Fig. 1. Double Tee junction.

The aim of this study is to determine a law of imperfect mixing with the help of high CFD simulations. By injecting a tracer through one entry (Fig1: In2) of the double-Tee, we want to know how it will spread into the outputs depending on the velocities as well as the distance L between the double-Tee. In the simulation we put no contaminant for the inlet 1 and full concentration for the inlet 2.

2.2. Mesh adjustment

Two comparable meshes are used. One was done for ANSYS Fluent with a cut-cell algorithm and is approximately 800,000 cells. The other was done for Code Saturne and is a structured mesh of more or less 1,000,000 cells. Both have been tested for grid convergence on the cases where all inflows and outflows are the same and comparative results were found. More tests need to be performed for different values.

2.3. CFD

We divided the work in two parts depending on our materials. Internally, we have access to a calculation center with 40 licenses for Fluent. We have also been able to use the calculation center of Aquitaine (France) called MCIA [7] with a lot more resources but without any ANSYS/Fluent licenses.

Therefore laminar calculations have been performed by DNS with Code Saturne on the MCIA while the Turbulent calculations have been made on the internal calculation center with Fluent.

3. Design of experiment: Interpolation and Delaunay triangulation method

3.1. Design of experiment

It was determined in previous studies that for Re>10,000 no further change in behavior is observed. Additionally, it was seen that after 20 diameters for the length between 2 Tees complete mixing occurs. A discussion with operating partners of SMaRT-Online[WDN] [11] has permitted us to fix the low boundary for distance between Tees. Indeed, crosses and double Tee junctions can't be compared easily because some space is needed to put in a valve in most cases. Therefore we have chosen the domain for the parameters of the Table (1):

Table 1: parameter domain

Factors	Low level (-)	Mid level chosen	High level (+)
Reynolds number between Tees	1 000	5 000	10 000
Distance between Tees	5*Diameter	10*Diameter	20*Diameter
Inlet velocity percent	0	50	100
Outlet velocity percent	0	50	100

To complete the study, we chose to make at least 3 experiments for every factor; as CPU time is long to get the stability, 81 simulations have been carried out. Additionally, we take advantage of control point simulation to get more reliable results in concordance with the Kriging interpolation and Delaunay triangulation.

3.2. Kriging interpolation

For making multi-dimensional inference, we use in this research the well-known *Kriging method* or *Gaussian Process Regression* [8] in geological sciences... This is a minimum variance method based on the definition of a probability distribution at each of the *n* sample points x_i. A spatial inference can be calculated for any point x_0 of the domain as a linear combination of these *n* points:

$$\widehat{Y}(x_0) = \sum_i^n \omega_i Y(x_i) \tag{1}$$

The weights ω_i are computed by assuming stationary state for first and second moments. This results in a constant mean for all variables and a correlation between two variables that only depends on the distance between them. The usual chosen form of correlation is the following:

$$\rho(d) = e^{-\theta \cdot d^p} \tag{2}$$

With *p* between 0 and 2 (optionally fixed) and theta a shape parameter. When *p* is chosen as 2, the correlation is named *Gaussian* and a Least-squares problem may be solved. In a more general case, θ and *p* can be fitted using

Maximum Likelihood Estimation (MLE) (Biles *et al.* (2007)). If the prior information is well chosen, this method is expected to be the best linear unbiased estimator (BLUE) [8]. In this study p was chosen as 2 and the library DACE [9] was used in Matlab.

3.3. Delaunay triangulation

DNS and LES simulations are computationally demanding, therefore a method is needed to find the best point of simulation. One well-known method is the Latin-square design consisting of dividing the space into a fixed number of squares and then randomly picking points in each square. However, for computational simulation, it has the drawback of selecting an unstructured set of points and it is not optimal to improve the interpolation fitting.

In this study we have selected the Delaunay triangulation method. This method has been used for the FFAST project [10] to improve a domain-decomposition. It was made to enrich the database of principal components analysis basis functions used in oscillating airfoils in a compressible flow context.

The Delaunay triangulation method and its dual the Voronoï diagram method are usually used for space partitioning. Here it is used to determine new points of simulations by a greedy algorithm:

- For each point of the design plan, calculate the difference between its value and the interpolated value at that point if it is not taken into account;
- For every Delaunay triangle (dual of Voronoï diagram) calculate the sum of the error of its vertices multiplied by its area, vertices being the points of the design plan.
- The best point candidates to include in the design plan are the centers of gravity for triangles with the highest weight;, then, in this research, the selected point is the closest point with rounded coordinates, more convenient for simulation.

A simple example is given in the Fig. 2, taking into account 9 points, which are given in Table 2:

Table 2: Delaunay method example points and corresponding errors

f(x,y)	x = 0	x = 1	x = 2	E(x,y)	x = 0	x = 1	x = 2
y = 0	1	0	1	y = 0	1.75	1	1.75
y = 1	2	2	2	y = 1	0.57	0.53	0.57
y = 2	3	3	3	y = 2	0.70	0.48	0.70

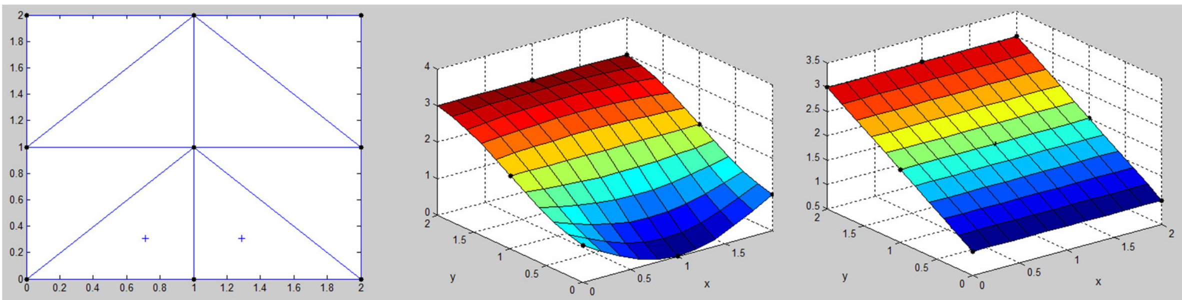

Fig. 2. left) Delaunay Triangle; center) full interpolation; right) interpolation without point (1,0).

The method will divide the space in 8 triangles of equal area. The maximum error is found on the points (0,0) and (0,2) equal to 1.7. In this case, the two-bottom triangles will most likely be chosen for new simulations (blue cross). The method detects the point most problematic, here the only point not in the plan z=x+1, and refines around it.

4. Results

4.1. Imperfect mixing law

The imperfect mixing law is computed from the table 3 of results of the simulations. The Kriging method is used to interpolate any value inside the range. Extrapolation out of range is not recommended and more research needs to be carried out there.

Table 3 gives a non-exhaustive list of the simulations performed. The first column is the distance between Tees (in diameters), the second is the average Reynolds number (in the center of the pipe), the third column is the Reynolds percent of inlet 1 (straight inlet see Fig. 1) from the last one, the fourth is for the outlet 1 (%In2 and %Out2 can be found from 100 - %In1 and 100 - %Out1 respectively). The last two columns give the repartition of contaminant for outlet 1 and 2 averaged in time. Indeed LES and DNS simulations are transient and therefore results need to be averaged for a sufficient period of time when converged. For the interpretation of results, it is worth to recall that 100% of the contaminant comes from inlet 2 and 0% from inlet 1.

Table 3: CFD Simulation results (non exhaustive)

Distance (in Diameter)	Reynolds	%In1	%Out1	%mean Out1	%mean Out2	distance (in Diameter)	Reynolds	%In1	%Out1	%mean Out1	%mean Out2
5	1000	20	20	21.6	78.4	5	5000	50	50	60	40
5	1000	20	80	81.1	18.9	5	5000	50	70	80	20
5	1000	80	20	54.8	45.2	5	5000	70	30	44	56
5	1000	80	80	86.3	13.7	5	5000	70	50	66	34
5	1000	30	30	30.1	69.9	5	5000	70	70	82	18
5	1000	30	70	71.7	28.3	5	10000	50	50	62.5	37.5
5	1000	70	30	58.8	41.2	5	10000	50	70	82	18
5	1000	70	70	93.4	6.6	5	10000	50	30	39.4	60.6
10	1000	20	20	21.5	78.5	5	10000	70	50	69	31
10	1000	20	80	81.5	18.5	8	5000	30	30	31	69
10	1000	30	30	32.5	67.5	8	5000	30	50	50	50
10	1000	30	70	70.5	29.5	8	5000	30	70	70	30
20	1000	20	20	20	80	10	5000	0	0	30	70
20	1000	20	80	80	20	10	5000	0	0	70	30
5	5000	20	20	20	80	10	5000	0	0	40	60
5	5000	20	80	79	21	10	5000	0	0	81.5	18.5
5	5000	30	30	29	71	10	5000	0	0	64	36
5	5000	30	50	49	51	10	5000	0	0	50	50
5	5000	30	70	69	31	10	5000	0	0	74	26
5	5000	50	30	37	63	10	5000	0	0	34	66

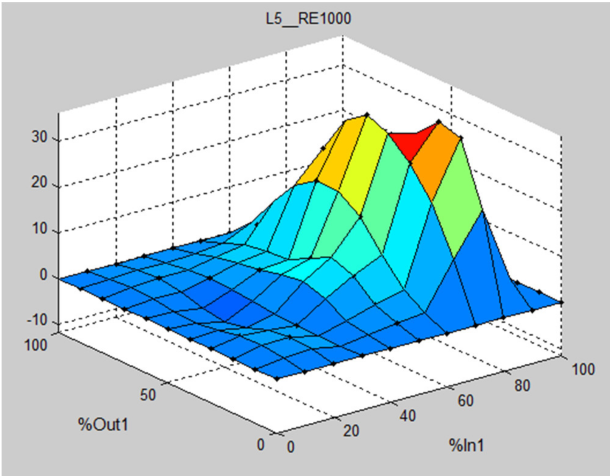

Fig. 3: Result for distance = 5D and Reynolds = 1,000

An interpretation of these results can be found when fixing 2 parameters. In Fig. 3 the distance is fixed to 5D and the Reynolds number is 1,000. It shows the difference from the complete mixing plan (Z=%Out1) to the result found in the simulations.

The difference is up to 30%, and therefore can't be neglected. It can also be seen that for %In1<50, that is when the straight inlet is dominated, the mixing law is more or less complete. A peak is visible with its top around %In1=70 found in every configuration.

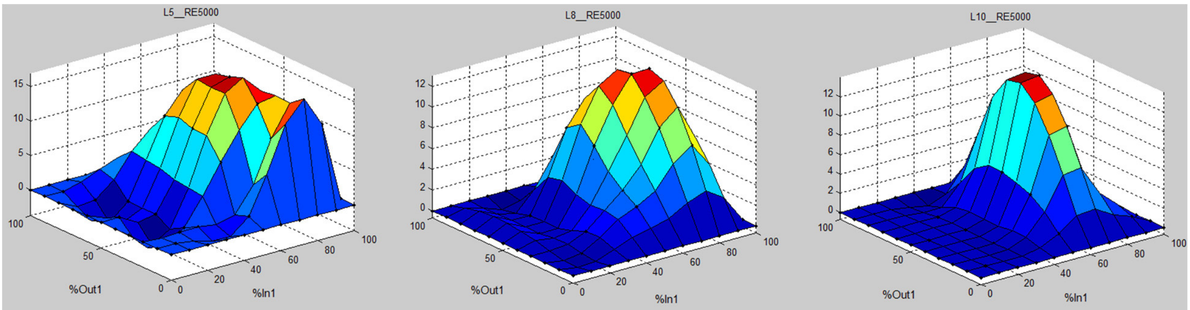

Fig. 4: Result for Reynolds = 5000, left) 5D, center) 8D, right) 10D

Fig. 4 shows the result when the Reynolds number is fixed at 5,000 and the distance is increased from 5D to 10D. It can be observed that there is a peak situated in the right part (when the straight inlet is dominating). The effect on increasing of distance between the two Tees looks to be a reduction of the peak in height and width. More simulations are needed for the case 5D as well as tests for grid convergence when the straight inlet is dominating (%In1>90).

A remark can be made concerning the boundary conditions: Contrary to previous studies, the boundary conditions are fixed for the complete mixing case. Indeed previous studies [2,3] also took these conditions for the left, bottom and top conditions but not for the right boundary condition (%In1 = 100). Around this last one the inlet 2 is almost closed and therefore almost no contaminant enters, however its repartition at the outlet is not clear. The simulations tend to show that it is complete mixing and therefore it was fixed in this study as such.

4.2. Simulation design plan results

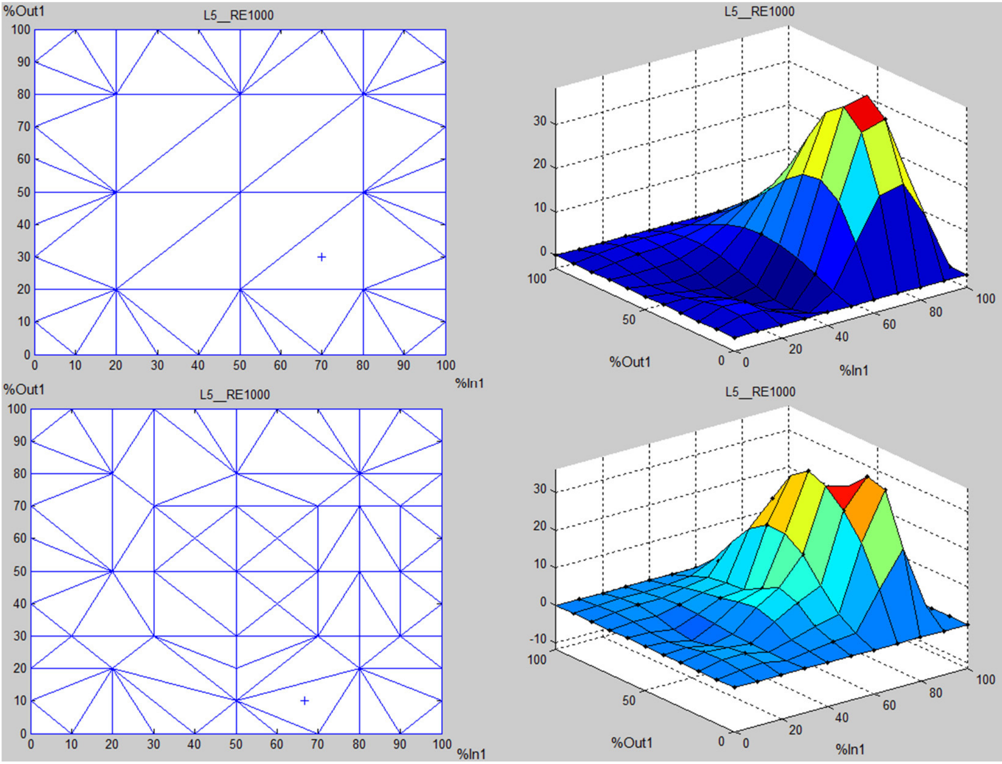

Fig. 5: Delaunay triangulation example for distance = 5D, Reynolds = 1,000: top) before, bottom) after 5 simulations chosen by Voronoï method

Table 4: Voronoï points for distance = 5D, Re = 1,000 case

Number	%In1	%Out1	Mean error	max error	number	%In1	%Out1	Mean error	max error
0	20	20	13,2	18,7	6	90	30	8,0	28,3
0	20	80	13,2	18,7	7	80	30	4,9	27,2
0	50	50	13,2	18,7	8	90	50	3,3	9,0
0	80	20	13,2	18,7	9	90	70	2,9	8,2
0	80	80	13,2	18,7	10	70	50	2,9	9,9
0	50	20	13,2	18,7	11	50	30	3,7	9,9
0	50	80	13,2	18,7	12	50	70	2,7	6,4
0	20	50	13,2	18,7	13	50	10	3,0	6,6
0	80	50	13,2	18,7	14	40	60	3,0	7,1
1	70	30	11,0	15,6	15	30	50	2,7	7,1
2	30	30	8,8	14,6	16	60	40	2,8	6,7
3	60	60	8,3	20,7	17	80	70	2,4	5,9
4	30	70	7,3	16,4	18	10	30	2,3	6,0
5	70	70	6,0	18,0					

In the example of Fig. 5 the Delaunay triangulation method has been used. On the left can be seen the Delaunay triangles partitioning the domain space, the blue cross define the new point of simulation to make.

Table 4 sums up the different new simulation points to consider found for the case where distance = 5D and Re = 1,000. The first column refers to the order of the simulations made given the Delaunay method and the number 0 is for the initial simulations. The second and third columns give the percent of inlet 1 Reynolds and outlet 1 Reynolds to the averaged Reynolds number 1,000. Finally the fourth and fifth columns are the absolute errors, either averaged (sum on number of points) or maximum, of all the points simulated at each stage.

In Table 4, it can be observed that for both types of error, it is globally decreasing. The error can increase when a particular point is found, in this example (90, 30), but then the Delaunay method will search for points around that will decrease the global error. Fig. 5 on the left shows the points of Delaunay location (vertices of the Delaunay triangle). At the end the method concentrates the points where there is a need for more information, here in the right part, when the straight inlet is dominating.

This justified the use of the Delaunay method for this study where each simulation cost a lot of computing resources.

5. Conclusion

In this paper, the imperfect mixing at double-Tee junctions has been studied through the use of high CFD simulations. Two software solutions have been used, Code Saturne for direct numerical simulations of laminar state and Fluent for turbulent cases using LES scheme.

Cost of computing justified the use of the Delaunay method to enhance and supplement the simulation results. A high interpolation scheme, the Kriging method, has been used in concordance with the Delaunay searching greedy algorithm for new points of simulation.

The results showed that there is not complete mixing inside our case study domain. When the straight inlet is dominating the results are close to perfect mixing. However a peak is likely to happen around the point 70% at Reynolds inlet 1 and 70% Reynolds outlet 1 and can't be neglected.

Finally it has been shown that the Delaunay triangulation automatic procedure is a good and simple method to find new points of simulation with efficient reduction of the interpolation error.

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