1. Introduction

Nowadays, research in microscale applications is gaining increasing interest, as can be seen in fields such as electronic engineering [1], 3D printing [2] or biomedicine [3], amongst many others. Despite their advances, the technology and resources needed to develop new designs may be a drawback for reduced scale engineering testing. To overcome this difficulty, computational methods represent a lower-cost tool than experimental testing in most applications. To develop and test many designs without the need of physically construct a prototype is an important advantage in design engineering. An example of application is the design of micro heat exchangers (MHE), which can incorporate elements to promote mixing by vortex shedding and can be constructed as LOC device (Lab On Chip). LOC mixing devices are portable reduced-scale lab devices that require small fluid consumption and provide a fast response feedback. Vortex shedding can be used in these devices for mixing processes, since this mechanism is widely used in applications such as the automotive [4], chemical and biotechnological [5] industry.

In this work, we aim to predict computationally the behavior of a vortex shedding-based passive mechanical micro heat exchanger (MHE). The MHE consists of a rectangular pillar structure in the centreline of a microchannel, which has two parallel flows coming into the
channel at different temperatures. The objective is to obtain the best thermal mixing between these flows by means of vortical structures. Concretely, the purpose of this investigation is to predict for which geometric&flow regime configurations vortex shedding appears, since not all feasible configurations experience this feature that promotes mixing. To carry out this study, this work is focused on the investigation of the effect of the Reynolds number ($Re$), the blockage ratio ($BR$), and the longitudinal aspect ratio ($AR$) in the generation of shedding. For each $BR$ and $AR$ configuration, there is a critical value of the Reynolds number, $Re_c$, above which the flow begins to oscillate and leads to the desired vortex detachment.

In fluid dynamics, vortex shedding is an oscillating flow, due to the collision between a flow fluid, for example air or water at certain speed, and a body at a specific location [6]. When the collision takes place, the flow separates, which sheds signature vortices from the structure and forms a “vortex street”, called von Kármán street [7]. Vortex shedding may or may not be beneficial to a specific application. For instance, a frequent engineering phenomenon of vortex shedding is Vortex-Induced Vibration (VIV). VIV has been considered in large constructions such as bridges, chimney stacks or in vehicle design processes. VIVs are oscillations caused by an object in a fluid flow. The vortices created push the object into different directions in a vibration-like basis, what perturbs the flow wake downstreams [8]. Although it is not the aim of the present work, the VIV can be applied in heat transfer applications such as [9], where they managed to improve heat transfer in a channel flow with heated walls supported by vortex-induced vibration, achieving a 90% increase in heat transfer compared to a normal channel. In [10] it was pointed out that the heat transferred from a vibrating cylinder was enhanced when Reynolds number had a value over 400. Finally, in [11] was achieved an important enhancement of the heat transfer at low Reynolds number.

In a MHE mixing two fluids at different temperature, if vortex shedding intensity is increased, the mixing will be enhanced and therefore more optimal and efficient. To promote vortex shedding, one can aggregate static objects or moving devices to perturb the flow. These enhancement techniques can be classified into passive and active. Usually, in passive techniques the channel is modified by modifying its surface, creating grooves or including objects as obstacles. However, active techniques incorporate moving elements and these elements consume additional power. The advantage of using a passive technique is that it does not consume power since the object is static [12]. Therefore, in the present investigation, passive techniques have been used, especially because at microscale to place moving objects can be cumbersome and static objects provided successful results in the literature [13].

Many studies have already been carried out on heat transfer based on the vortex shedding generated by flow separation around a pillar or cylinder. Some of these studies have been focused on finding the best shape for the object the fluid collides with to generate vortex shedding, as hexagonal cylinders in [14] or with a square cylinder in [15]. Other investigations have focused on the use of vortex shedding for heat transfer from heated cylinders, as for instance in [16], or in the mixing process in 3D mixers with T and DT shape geometries where the mixing index is analysed [17]. The most common applications that have been studied about heat transfer are those related to fluids passing through an object at different temperatures, as can also be seen in [18] and studies related to unconfined flows [19]. However, it is true that in cases where vortex shedding is used for chemical mixing applications, it is unusual to find studies in where the $AR$ and $BR$ are varied, as only done in [13]. In the rest of the literature, the investigation has been focused on varying the $AR$ or the $BR$, but not both jointly, as seen for instance in [20] or in [21].

Being able to predict the vortex shedding is crucial, because it improves fluid mixing and permits to obtain better designs. For mixing purposes, one would not be interested in configurations that do not lead to vortex shedding. Thus, flow behavior prediction may improve design optimisation frameworks. The prediction of vortex shedding has already been carried out
in studies such as [22] to calculate the magnitude and spatial distribution of fluid stresses in heart valves, or in [23] using Deep Learning, which is a field of Machine Learning (ML). Generally speaking, ML algorithms can increase the knowledge of the flow domain that we want to study, optimising the flow and keeping control with support from automated tasks [24]. Random Forest (RF) is a ML predictor model introduced by Kam [25] which consists of a set of predictor trees, it has a high level of classification accuracy, and usually tolerates noise and outliers [26]. Some researchers have already tested the RF in fluid dynamics applications, such as [27] in where the non-negativity of the eddy viscosity, the isotropy of the eddy viscosity, and the linearity of the relationship between the Reynolds stresses and the mean strain rate were investigated. It was demonstrated that the RF algorithm was the one that had the lowest class-averaged error. In [28] it was predicted Reynolds stress discrepancies in different flows using RF, evaluating flows at different states. Due to those factors, RF is an adequate classification technique to implement in this work.

In addition, correlation models can be constructed to approximate the response of the complex system in a simplified way. These represent a quick tool to estimate the value of a quantity of interest not requiring a simulation or experimental run. It is common to see correlation models related to heat transfer [18]. But generally speaking, correlation models are not suitable to know if a certain configuration will produce a vortex shedding, since this would be a classification problem and correlation models are used for regression analysis. In this work, correlation models are used to predict the values of the critical Reynolds number above which vortex shedding appears for a certain geometric configuration.

This paper is divided into different sections as follows. Section 2 introduces CFD simulation and describes the regression and random forest classification in Machine Learning. Section 3 explains the prediction of the vortex shedding and the prediction of the critical Reynolds number. To finish, in Section 4 the conclusions are given.

2. Numerical and Theoretical Aspects

2.1. CFD simulation

The engineering problem under study consist of a vortex shedding-based micro heat exchanger (MHE) that enhances mixing between two fluids. A sketch of the geometry is shown in Figure 1. The geometry is basically a pillar confined in a microchannel of width $H$, with a blockage ratio $BR = \frac{h}{H}$ and the longitudinal cylinder aspect ratio of $AR = \frac{l}{h}$. According to the position of the system of coordinates shown in Figure 1, the pillar positioning is located at a distance of $L_u = H$ from the microchannel inlet, and $L - (L_u + l)$ from the microchannel outlet, with $L = 5H$ the microchannel length.

![Figure 1. Sketch of the micro heat exchanger. Image taken from [13].](image)

The problem is governed by the Navier-Stokes equations, which for a 2D domain and incompressible flow can be written dimensionless as:

$$\nabla \cdot \mathbf{v} = 0,$$
\[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{v}, \]  
with \( \mathbf{v} \) the velocity vector \( \mathbf{v} = (u, v) \), \( p \) the pressure, \( Re \) the Reynolds number, \( Pr \) the Prandtl number and \( \theta \) the dimensionless temperature. The Reynolds number is defined according to \( Re = UH/\nu \), with \( \nu \) the kinematic viscosity and \( U \) the mean inlet velocity. In the present work \( Re \) is low, ranging between 120 and 200, thus the flow is laminar (viscous forces are more dominant than inertial ones). Since the main interest in the present work is to address the performance of the vortex shedding-based mixing, and not the fluid-dependence mixing, a constant high value of the Prandlt number is imposed to the working fluids under the assumption of negligible effect of temperature in their fluid properties: \( Pr = \nu/\alpha = 10^4 \), with \( \alpha \) the thermal diffusivity. If the \( Pr \) was low, the heat transfer would be dominated by the diffusivity of the fluids, and the impact of the geometry variations and flow velocity would be reduced and hard to quantify.

The governing equations require specific boundary conditions in order to solve numerically the problem. The inlet consists of a fully-developed parabolic profile, whose expression for a laminar channel flow is given by the dimensionless axial velocity: \( u/U = 6\left(\frac{1}{4} - \left(\frac{y}{H}\right)^2\right) \). The velocity component in the \( y \)-direction is zero: \( v/U = 0 \). Also, the inlet consists of two fluids at different temperature. Their temperature \( T_i \) (\( T_1 \) is the cold fluid, and \( T_2 \) is the hot one) is made dimensionless by \( \theta_i \):

\[ \theta_i = \frac{T_i - T_1}{T_2 - T_1} = \frac{T_i - T_1}{\Delta T}, \]

with the inlet boundary condition set as:

\[ \theta = \theta_1 = 0 \text{ at } x = -(L_u + l/2), \quad 0 < y \leq H/2, \]
\[ \theta = \theta_2 = 1 \text{ at } x = -(L_u + l/2), \quad -H/2 < y \leq 0. \]

At the outflow of the microchannel, the flow has to remain unperturbed for a correct simulation, thus the gradients for the transported quantities \( \phi \) must be set to zero value (\( \partial \phi/\partial x = 0 \)) and atmospheric pressure is imposed at the outflow. Regarding the heat fluxes between the flow and walls, these have been set to zero (adiabatic surfaces). This boundary condition is imposed onto the four walls of the pillar and both walls of the microchannel as \( \partial T(x_s, y_s; t)/\partial n = 0 \), where \( n \) is the coordinate normal to the surface and \((x_s, y_s)\) is the location at these surfaces. Also, the walls are under non-slip conditions, i.e. velocity is zero at the surface and boundary layer is formed: \( v(x_s, y_s) = 0 \).

To solve the problem numerically by the finite volume code, the domain must be discretised spatially and temporally, and specific numerical schemes must be used. After a mesh convergence analysis (see [13] for details) the domain is discretised with a \( \Delta x = \Delta y = 0.004H \). This makes results mesh independent. This grid size also allows to solve the Batchelor’s mixing length scale \( \Gamma [29, 30] \), which is of \( \Gamma \sim 0.01H \) size in the present study. The SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) [31] is used to couple the velocity and pressure equations and second order schemes are used for high accuracy in the numerical solution. The temporal discretisation has been selected to always satisfy the Courant-Friedrichs-Lewy number to be lower than the unity value. The validation of the numerical simulations is shown in Figure 2. In such figure, the validation is carried out for the Strouhal number of the lift coefficient, \( St_{cl} \), and the time-averaged drag coefficient, \( \langle Cd \rangle \), at different \( BR \) with fixed \( AR = 1 \) and \( Re = 100 \).
2.2. Regression and Random Forest Classification in Machine Learning

There are many scenarios where a scientist needs to infer the value of a quantity of interest (QoI) upon previous collected data. The action of estimating this quantity is popularly known as predictive modelling in Machine Learning literature. With the objective of prediction, one can find two important groups: regression models and classification models.

Regression modelling are a supervised modelling approach that intends to use existing data (training data) to construct a function that aims to model a continuous output variable [33]. For a given input, the output is a numerical value. The function that creates an empirical relation between the observed and actual data can be constructed as a linear or non-linear relationship.

Let consider a linear regression. For each observation $Y_i$, a set of coefficients $\beta_j$ must be found to model the relationship between the two variables $Y$ and $X$:

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + ... + \beta_N X_i^N + \epsilon_i,$$

where $\epsilon_i$ is the error in the regression (which follows a normal distribution of mean equals to zero). If its value was zero, that would mean that the regression would have a perfect fit. This expression can be written in matrix form as

$$Y = X\beta + \epsilon,$$

with $\beta$ the vector of coefficients, $\epsilon$ the vector with errors $\epsilon_i$, $Y$ the vector with the $Y_i$ observations of the variable to predict, and $X$ the design matrix with $i$ rows and whose number of columns is the number of $\beta_j$ coefficients to estimate (for instance, for a polynomial fit of order $N$ the number of columns is $N + 1$). The last step thus consists on estimating the value of the coefficients $\beta_j$.

A popular approach is the use of the Least Square Method. This consists of estimating the $\beta_j$ coefficients that minimise the regression fitting errors. Since the errors can be defined as

$$\epsilon = Y - X\beta,$$

the objective is to minimise its “square” value:

$$\min[\epsilon^T \epsilon] = \min[(Y - X\beta)^T (Y - X\beta)],$$

where superscript $T$ indicates the transpose. In order to calculate the minimum, one has to derive the expression and make equal to zero. This yields the following:

$$-2X^T(Y - X\beta) = 0,$$
and thus the solution to the least square problem is

$$ \beta = (X^T X)^{-1}(X^T Y). \quad (10) $$

Whilst regression models do focus on predicting a continuous variable, classification models are predictors whose aim is to predict a categorical variable. When the categorical variable has only two classes, the problem is known as binary classification. Some sort of regression models can be also applied for classification, as for instance the Logistic Regression [34, 35], since its output is a continuous parameter between 0 and 1 that reflects a probability. By establishing a threshold, the output can be used for classification. In the present work, the classification model to be used is the Random Forest (RF) [36]. A RF classifier is basically an ensemble of several decision trees. The method performs a bootstrap randomised sampling on the training dataset in order to train several decision trees that will be ensembled. This bootstrap method can be developed with replacement, that means that if the dataset is reduced, the same samples can be re-utilised to train the trees.

Let define as $\Theta$ the vector of hyper-parameters $\Theta_k$ that define the RF algorithm. Since each tree $h_k$ is grown using each random vector $\Theta_k$ and the training data set $D_t$, this results to

$$ h_k(X) = h(X, \Theta_k). $$

In [36], a RF classifier is defined as “a classifier consisting of a collection of tree-structured classifiers $\{h(X, \Theta_k)\}, k = 1, ..., M\}$, where the $\{\Theta_k\}$ are independent identically distributed random vectors and each tree casts a unit vote for the most popular class at input $X_i$”, where $M$ is the number of trees. Although RF can be used either for regression or classification, the definition of the prediction is defined differently. As aforementioned, RF is an ensemble of several models. In a regression problem, the selection of the predicted value amongst the performance of several regression models (say a total number of models $M$) can be simply the average of all the predicted outputs. However, in a classification problem, the predicted class $C_{RF}^{D_t, \Theta_1, \Theta_2, ..., \Theta_M}$ upon the $M$ decision trees must be selected as the majority vote of a class $c \in Y$, that is [37]:

$$ C_{D_t, \Theta_1, \Theta_2, ..., \Theta_M}^{RF} = \text{argmax} \sum_{m=1}^{M} (h(X, \Theta_m) = c). \quad (11) $$

For ensembled predictors, as the RF, the sampling method employed to construct the intermediate models left parts of the original sample unused. These can be utilised to generate new measures of error. The Out-Of-Bag (OOB) error is a generalisation error that arises from evaluating the intermediate models (in RF, the decision trees) that did not include the left-out samples in their bootstrap sampling process [38, 37]. Since samples not used in training are used for test, the OOB error can be somewhat considered a validation test. This makes unnecessary to separate the data into training and test datasets. If additional testing is desired, the most popular tests in the literature are the $k$-fold cross-validation tests. The $k$-fold cross-validation process splits the training data into $k$ folds and next the classification model is trained with $k-1$ folds and tested on the unused $k$-th fold. This is a useful test for overfitting, since let us test if the number of selected features is adequate. For the performance of the classification model, a reference measure must be used. In classification problems, the ability to predict by a classification model is reported by means of the Area Under the Receiver-Operating Curve (AUC-ROC, AUROC or simply AUC) [39]. The ROC curve is a graphical representation of the sensitivity and specificity of a predictor, and it is thus probability-based. The area AUC enclosed by this curve is used as reference for the performance of a classificator. This parameter shows how accurately the predictor differentiates each class. Thus, $AUC = 1$ means that the predictor is able to classify correctly all classes. A value of $AUC = 0.5$ means that the predictor performs as a random decision, i.e. as coin tossing.
3. Results
The interest on predicting whether a configuration may or may not lead to vortex shedding is based on the mixing performance. In Figure 3 is shown a MHE with strong intensity, low intensity and without vortex shedding. It can be visualised the strong importance of the geometry for a given flow regime and how important is to predict whether a certain configuration will be of interest to avoid irrelevant simulations or experimental prototyping.

![Figure 3. Examples of expected heat transfer performances of the MHE.](image)

3.1. Predicting Vortex Shedding
For each MHE design, there are two possibilities: the design leads to a steady state solution or leads to a oscillatory behaviour with vortex shedding. Thus, the action of identifying which type of performance corresponds to each configuration is a binary classification. A Random Forest (RF) algorithm is trained for this purpose. The data used to train the RF classifier consists of a total of 80 simulations, where the class variable to predict is vortex shedding, being 0 (no vortex shedding) or 1 (vortex shedding). The 80 simulations correspond to all possible combinations of $Re = \{120, 140, 160, 180, 200\}$, $BR = \{0.2, 0.3, 0.4, 0.5\}$ and $AR = \{0.125, 0.25, 0.5, 1\}$.

As RF is an ensemble of trees, the total number of trees has been guessed from the OOB error reported in Figure 3.1. Practitioners usually recommend to select the number of trees $M$ close to the value at which the OOB error remains nearly stable. However, there is no actual restriction (just in terms of computational resources) since convergence is expected, and some authors suggest that few hundred are enough [40, 38]. Can be observed that the OOB error is stable from $M = 400$ on, thus a total of $M = 500$ trees have been selected for the training of the RF algorithm. Must be pointed out that the OOB error can be reduced if additional samples are added by means of new CFD simulations.

Due to the fact that the number of features (parameters used for prediction) is quite low ($AR$, $BR$ and $Re$), the selection of the features to be randomly sampled in the bootstrap algorithm is fixed to 3. For RF and any classification algorithm it is important to control not only the
number of features, but also sample characteristics, such as if the size of the training data is reduced or imbalanced. In a bad case scenario, additional actions should be taken. The dataset is not notably imbalanced, with the minority class $VS = 0$ of 33.75% (there is not a solid consensus on this, but a dataset is frequently assumed to be highly imbalanced for minority class below a 10%). However, the size of the data set is 80 simulations only, and this obliges to use a replacement sampling in the bootstrapping technique.

The RF classifier that results from the discussed algorithm configuration is able to predict all cases without false negatives nor false positives, as illustrated in the confusion matrix in Table 1. The confusion matrix compares the predictor output (predicted value) with respect to the actual value (reference). This matrix shows that the RF classifier is an accurate tool for vortex shedding prediction in MHE. However, it must be noted that overfitting may obscure the real performance, being the classifier too adjusted to the specific training data. Although by means of the bootstrap method the RF is internally selecting kind of a “training and test” data, additional testing would be desirable. With only three parameters (features), overfitting is very unlikely. However, a 8-fold cross-validation test was also developed, as shown in Table 2. The 8-fold sampling has been split ensuring a level of stratification (the classes are balanced). Since all folds yielded nearly the same prediction measures ($AUC \simeq 1$), we can be confident with the predictor.

![Figure 4. OOB error of Random Forest algorithm versus number of trees.](image_url)

| Reference data | 0 | 1 |
|----------------|---|---|
| Predicted value | 0 | 27 | 0 |
|                | 1 | 0  | 53 |

**Table 1.** Confusion matrix for the Random Forest predictor.

### 3.2. Predicting the Critical Reynolds Number

As studied in the precedent subsection, a classification model can be constructed to predict which combinations of $Re$, $AR$ and $BR$ lead to oscillatory behaviour, which takes place surpassing a critical Reynolds value $Re_c$ for a given geometry: $Re_c = Re_c(AR, BR)$. However, this model
for this new objective, regression correlation models can be developed, as studied in previous works [13].

For this analysis, a two-step process is developed. As in Figure 5 can be observed that a straight line may be enough to cluster each group (vortex shedders and non-vortex shedders), the process is focused on obtaining this inverse problem solutions. First, a linear relation between \( Re_c \) and \( BR \) is sought for each \( AR \) value, of the form:

\[
Re_c = a_i BR + b_i, \tag{12}
\]

where \( a_i \) and \( b_i \) are the fitting coefficients for each case. Second, a new inverse problem arises in terms of modelling a global \( a \) and \( b \) constant, that allows to model \( Re_c \) as dependent on both \( AR \) and \( BR \). For this purpose, a third-order polynomial and a linear fit seem to be the best approach for \( a_i \) and \( b_i \), respectively, as depicted in Figure 6. For \( b_i \) a 2nd order polynomial fit would have fit slightly better, but a linear trend is clear and preferred for the sake of simplicity in the model. So the final empirical regression-based correlation model for \( Re_c \) is given by the expression:

\[
Re_c = -609.52 AR^3 \cdot BR + 533.33 AR^2 \cdot BR - 133.33 AR \cdot BR - 190.48 BR + 183.7 AR + 143.9, \tag{13}
\]

which is only valid within the range \( Re \in [120, 200], AR \in [0.125, 1] \) and \( BR \in [0.2, 0.5] \). The correlation model performance of the model suggested in Equation (13) is shown in Figure 5.

The characterisation of the \( Re_c \) by the model is as exact as only 1 case out of the 80 is grouped incorrectly.

Figure 5. Effect of Reynolds number, aspect ratio and blockage ratio on vortex shedding (VS).
The regression models found in this study allow to know the Reynolds number that must be surpassed for a given $AR$ and $BR$ in the design process of an efficient micromixer. Thus, in a constrained optimisation process, these functions could be implemented as constrains for $Re$. This may help optimisation algorithms, since if $Re$ below $Re_c$ are discarded, computational resources may be saved.

4. Conclusions
This investigation examines the use of mathematical models in the prediction of vortex shedding in micro heat exchangers (MHE), which consists of a rectangular cylinder positioned in the centreline of a microchannel with two fluids at different temperatures as inlet. The existence of an intense oscillatory motion downstream the cylinder has been utilised by several researchers in the development of micromixers, but it is not possible to know before construction whether a geometry and regime would lead to vortex shedding to promote mixing. The use of the suggested models can help engineers and scientists in the task of creating efficient designs with a data-driven tool. In constrained optimisation studies, these models can be used as non-linear constrain, to avoid sampling inefficient mixers (configurations without vortex shedding).

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