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Heterogeneous Approach in Reforming Batch Reactor Structure for an Improved Efficiency

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While numerous studies focus on homogeneity in increasing the utility value of a system, its feasibility and practicality are inconclusive; even with the possible limitations of a homogeneous approach, the potential of promoting heterogeneity is still overlooked. This paper reports that the use of partitions leads to the making of controlled thermal heterogeneity, where variance in flow direction and temperature is measured in terms of energy and mass imbalance. Moreover, through a qualitative analysis using Particle Image Velocimetry (PIV) and a quantitative analysis via a soft-sensing technique, the percentage change in temperature was shown to decrease from 58.0 to 21.8 % after four rounds of residence cycle. This gradual stabilization indicates the system's advancement towards a steady-state, where a maximum of 1.0 K temperature difference is observed to be retained. The novel approach of controlling the inner state of a space using partitions allows a single space to have multiple zones that each demonstrate appropriate conditions for a unique demand; thus improving the system's efficiency in terms of energy, space and time. This concept of heightening the system's performance via the promotion of heterogeneity using partitions is applicable in, but not restricted to, the industrial sector where thermal heterogeneity in a reactor can effectively cater to the simultaneous production of multiple outputs from one vessel.

1. Introduction

The endeavor to create a space that constitutes multiple environments is proven crucial as numerous demands can be met within the limited space and time. This idea of augmenting the utility value of a space by enabling numerous reactions to take place is applied in industrial reactors, such as fluidized bed reactors (FBR), where different levels of heat transfer occurring through walls or separators lead to the establishment of different reaction conditions (Tawfik et al., 2019). Such intentional differentiation of conditions affects the conversion rate and the stability of the catalyst, which allows for a controlled process variables and an effective fluid dynamic to be attained within the system (Landa et al., 2022). Likewise, reactive distillation columns with dividing walls are used to make multiple products from a single column (Speight, 2020) where the morphology of the column allows the selectivity of the reactions to be directly influenced (Chaniago et al., 2021). This system that employs physical separation within a space demonstrates energy efficiency and lower cost in yielding the products (Devaraja & Kiss, 2022). Moreover, the creation of an air-conditioned room with differing thermal environments is another daily example in the use of the aforementioned idea where numerous demands are met in one space (Xu & Peet, 2021). From these aspects, various conditioned space contributes to the heightening of efficiency in terms of cost and energy usage, not only in the industrial sectors but also in the commercial and residential sectors.
Despite having the ability to create a multi-conditioned space, the level of difference across the space, herein referred to as heterogeneity, cannot be intentionally set from the user's end in many cases. This inability to control the environment impedes the users from managing the speed, quality and direction of the desired reaction; ultimately compromising the reproducibility of the expected results.
With the evident limitation in controlling a heterogeneous space, this paper aims to explore the potential of partitions in initiating and sustaining a thermally heterogeneous space with a predictable amount of difference in temperature and flow directions. Normally, Computational Fluid Dynamics simulations are used to visually

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understand how heat transfers in a space (Tian et al., 2019) which is further analyzed to suggest the optimum setup of a space for maximum output (Lan et al., 2021). Deviating from this usual approach of conducting a Computational Fluid Dynamics simulation, this paper experimentally analyzed the heat flow and temperature change of a model space made of an aquarium. Additionally, by restricting the number of inflow and outflow to one, the creation of and the spread of heterogeneity across the space were assessed through mass and energy balance using Particle Image Velocimetry (PIV) and temperature sensing techniques, respectively. Overall, the parameters that demonstrate the most influence over the difference in temperature and flow directions are identified, where its manipulation suggests the possibility of quantitatively controlling the level of heterogeneity present in a space.

2. Flow analysis

To emulate a partitioned space with one source of incoming change, an acrylic partition of various heights was inserted into an acrylic tank of width 184 mm, length of 184 mm and height of 194 mm. As seen in Figure 1, the tank is equipped with a pair of nozzles, situated at the center and at the side of the tank to allow water to be supplied and vacuumed at a constant rate. By keeping the flow rate constant, the mean residence time (τ) of the system, defined as the average time that fluid stays in the space, is set to be approximately 6 minutes. The calculation of the apparent mean residence time is shown in Eq(1) where it takes the ratio between the tank volume (V) and the volumetric flow rate (Q).

$$\tau = \frac{V}{Q} \tag{1}$$

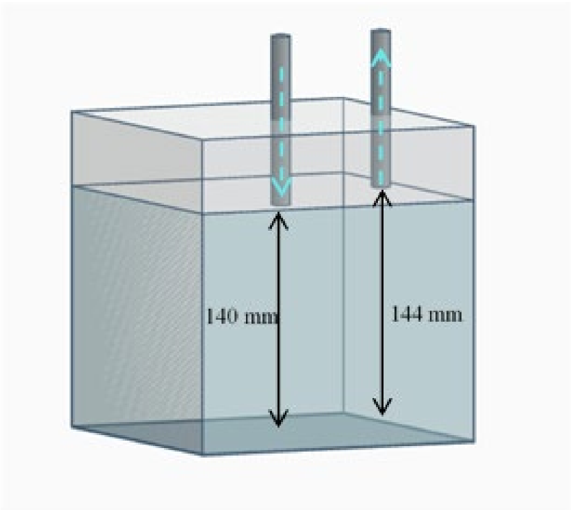


Figure 1: Experimental setup

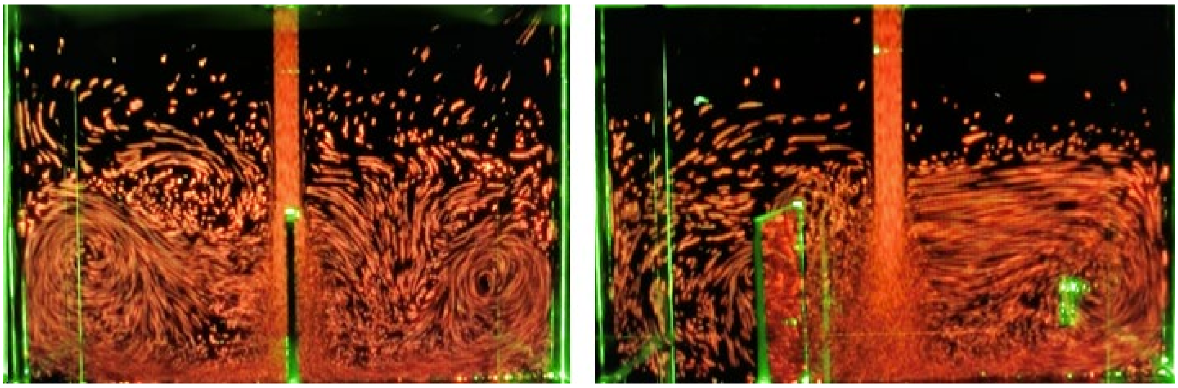
The impact of partitioning a space was investigated using a PIV approach, where the induced flow pattern was interrogated by capturing the trajectory of the tracer particles introduced into the system. As seen in Table 1, three different trials were executed to assess the influence of partition height and position in the flow direction, all while keeping the inflow conditions constant. Importantly, the heterogeneity in the flow pattern was assessed via a) its shape and b) intensity, where the shape is evaluated by the location of the created vortices, and the intensity is measured in terms of the mass balance of the accumulated tracer particles.

Table 1: Trial conditions

Trial Number	Partition Height (mm)	Partition Position	Inflow Rate (±10 mL/min)	Inflow Water Temperature (±0.4 K)	Tank Water Temperature (±0.4 K)
1	60	middle			
2	60	1/3 from left	700	10	35
3	90	1/3 from left			

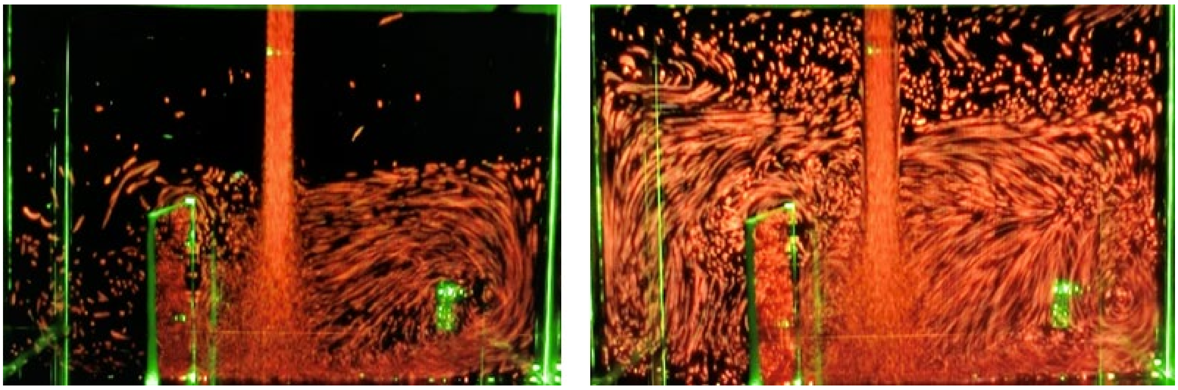
2.1 The effect of partition position

Trials 1 and 2 are compared to assess the level of influence the partition position has over the created heterogeneous space. As seen in Figure 2, the symmetrically divided tank shows homogeneous characteristics such as a mirrored flow shape and symmetrical flow intensity at the partition line, where equally sized vortices are found on the left and the right, alongside a congruent level of tracer accumulation on both sides. Conversely, the asymmetrically divided tank exhibits heterogeneous traits with vortices that are not mirrored, which is accompanied by a considerably low accumulation level of tracers on the left-hand side.
Interestingly, upon investigating the development of heterogeneity, the level of partition's influence changed over time for flow intensity, while it maintained its prevalence over the flow shape. In-depth, as seen in Figure 3, the unevenness in the spread of tracer particles, shown in red, decreases its characteristic as the intensity of redness on the left gradually increases to match that of the right. This weakening of mass imbalance indicates the loss of heterogeneity from the flow intensity perspective, caused by the inevitable overflow of particles. On the contrary, the position and the number of vortices do not change with time, proving the sustenance of the partition's influence over flow shape.



(a) (b)

Figure 2: PIV data of (a) trial 1 and (b) trial 2

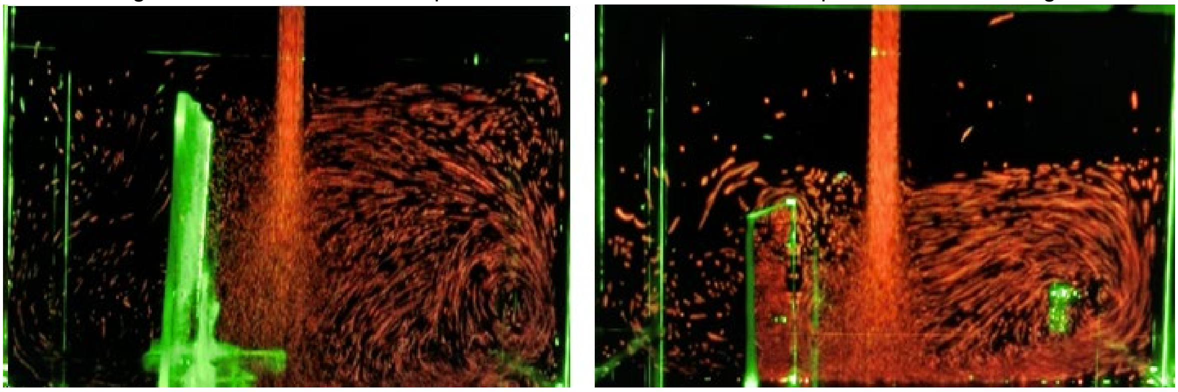


(a) (b)

Figure 3: Time lapse of trial 2 at the (a) initial 30 s and at (b) the 270 s timestamp

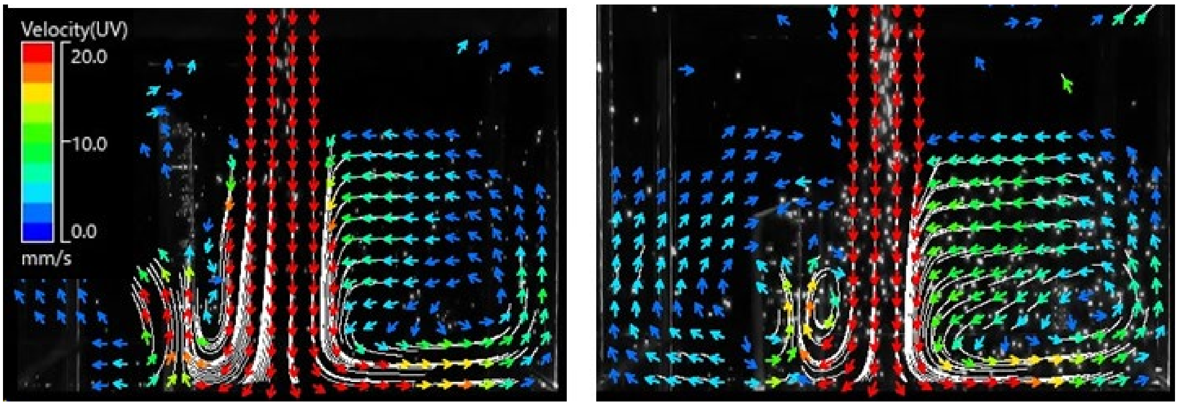
2.2 The effect of partition height

Next, the role of partition heights was assessed by comparing trials 2 and 3. Comparing the geometry of the space by using vortex position as an indicator, Figure 4 identifies the absence of the partition's influence over the flow shape as corresponding vortices are spotted at the same spots: one at the right of the tank and another beside the partition wall. Accordingly, the focus was shifted to the difference in flow intensity, where a software analysis (FlowExpert64, Katoken, Version 1.3.3) was conducted over the experimental data to minimize human error when tracing the minuscule particles. As a result, as seen in Figure 5, trial 3 with a higher partition had fewer particles being detected, as seen in the number of vectors, on the left of the partition than trial 2 with a lower partition. This indicates how the effect of changing the partition height manifests in the difference in resistance against the overflow of tracer particles to the side with no direct impact of external change.



(a) (b)

Figure 4: PIV data for (a) trial 3 and (b) trial 2



(a) (b)

Figure 5: FlowExpert software analysis of particle velocity for (a) trial 3 and (b) trial 2.

3. Temperature distribution analysis

The focus is now shifted to an energy balance approach with temperature change being evaluated. Considering the result of the PIV experiment, a thermally heterogeneous space was recreated by placing the partition at the 1/4 position from the left. Additionally, to evenly measure the temperature distribution, the tank was equally divided into three levels, where each level was further divided into 16 squares, as shown in Figure 6. An important point to note is the location of the partition at the E1, B1 points, and the consequent placement of the two separate thermocouples at E1 and B1 to measure the temperature of each side of the partition.

The thermocouples at the left of the partition expressed a higher temperature than its symmetrical point on the right as the cooling source of inflow is positioned above the C2 position. In addition, similar to the effect of overflow seen in mass imbalance, the level of heterogeneity shown in the form of energy imbalance decreases with time as thermal equalization occurs through induced and natural convection. More specifically, as seen in Figure 7, the largest temperature difference between the left and the right of the partition for both B1 and E1 is observed at the 90-s timestamp, where B1 experiences a temperature difference of 4.75 and 7.80 K, while E1 experiences a 5.35 and 7.40 K difference in the middle and the bottom layers. This gap eventually diminishes to 0.10 and 0.65 K for B1, and 0.30 and 1.00 K for E1 middle and bottom layer.

Despite the sharp decrease in temperature difference after the 90-s threshold, a measurable amount of difference is proven to remain even after 25 min, which is equivalent to 4 residence cycles. Additionally, the gradual flattening of the graphs in Figure 7 reflects the stabilization of temperature, where the percentage change in the temperature difference decreases from 58.0 to 21.8 % in just 4 residence cycles. This trend of decrease in the magnitude of change suggests the system's advancement towards a steady-state, where the residual temperature difference emphasizes the space's ability to reserve a certain level of heterogeneity.

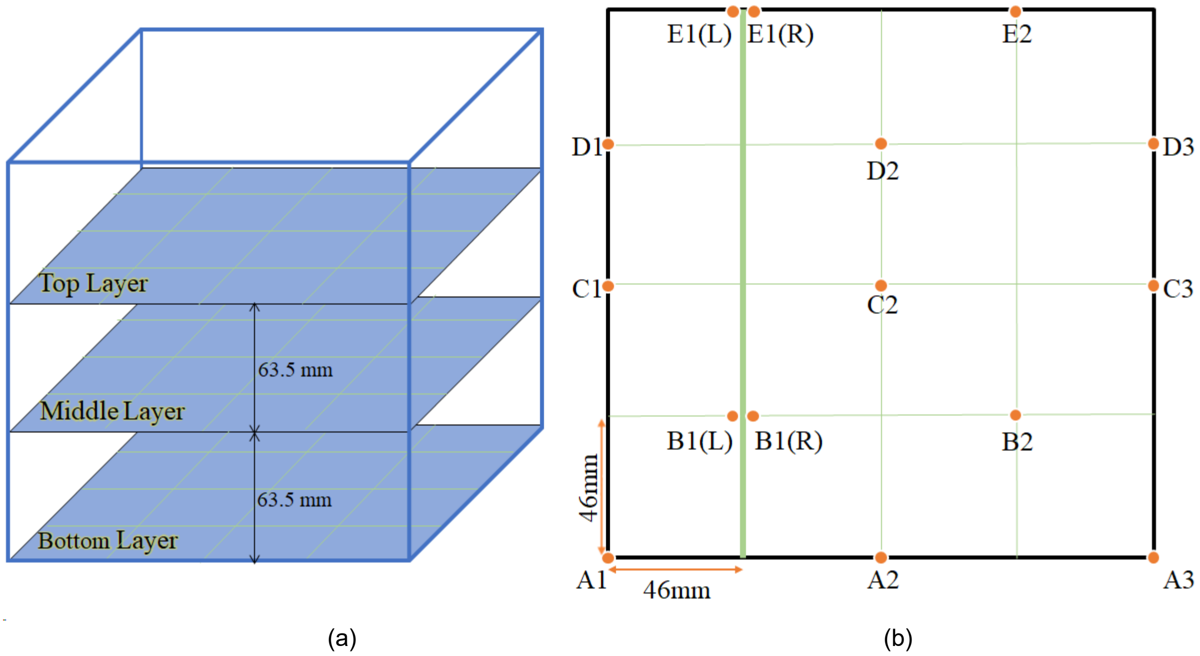


Figure 6: (a) Front-view and (b) bird's-eye-view of the thermocouple setup

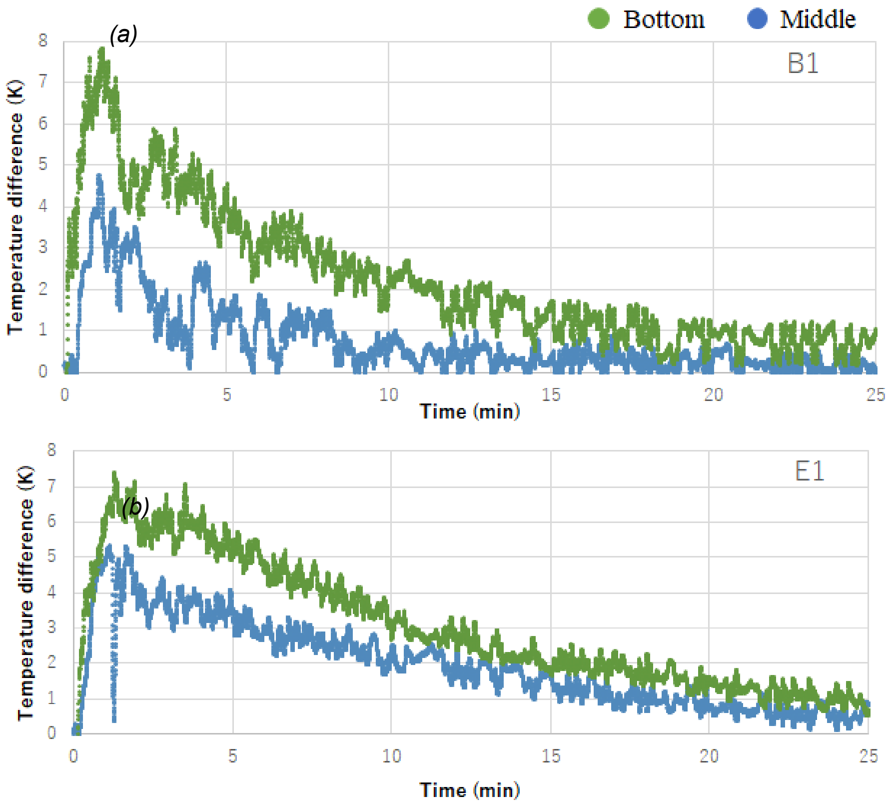


Figure 7: Temperature difference between the left and right of the partition over four retention cycles at (a) B1 and (b) E1.

4. Discussion

To increase and extend the influence of partitions, the physical and thermal mixing that happens across the partition site must be minimized. The most intuitive approach is to place a high partition far away from the source of change to delay equalization, or to have several partitions in a space as an attempt to confine the impact of change to one section. A more complex approach includes the addition of an external force, such as a circulator, that will mechanically repel the fluid from overflowing. Moreover, if a more passive approach that requires less energy input is favored, altering the shape of a partition that will physically obstruct the flow pattern, such as a hooded partition, is suggested.

Extrapolating the idea of manipulating heterogeneity, the creation of ‘appropriate' zones within a space through the use of partitions is proposed as a solution to the issue of having multiple demands existing at once. For instance, by differentiating the temperature and the molar concentration of reactants across an industrial reactor, the rate and the direction of the reactions taking place in a single vessel, in other words, the reaction rate constants of the system, can be controlled. By controlling the state of each zone to fit the optimum conditions of a unique reaction, the product yield is heightened in terms of both quantity and quality. Moreover, by extracting the products from the vessel as it is being made, the issue of the established heterogeneity decreasing will be prevented. This additional step acts to sustain the initial concentration gradient, ultimately postponing the system from reaching chemical equilibrium. Another application example that takes a more commercial approach, is the use of partitions in the making of many “comfort” zones in an air-conditioned room, where the ironic subjectivity of the word comfort acts to strengthen the idea of having a thermally heterogeneous space.

5. Conclusions

The ways in which partitions affect heterogeneity was investigated in this paper, where the two parameters of partition position and size was shown to impact the development of heterogeneity. First, the position of the partition showed permanent dominance over the orientation of the space, as assessed by the level of symmetry in the vortex observed through the PIV system. Second, the size of the partition showed time-dependent influence over the system's strength of resistance against equalization in mass and energy imbalance. Although the influence of partition size decreases with time, a portion of its initial impact shows to persist in the system as temperature and/or concentration difference was observed after multiple rounds of residence cycle. As the system progresses into a steady-state with no further net changes, the retained heterogeneity is measured as system's sustainability. Responsively, understanding how much temperature difference and concentration gradient remains over time is made essential in measuring the utility value of the system.(Landa et al., 2022)

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