Abstract: Global regulations for emission reduction are continually becoming stricter, and conventional catalytic converters may be efficient in the future because of their low conversion efficiencies at cold-start. In this study, to overcome the performance limitations of conventional catalytic converters, a three-dimensional (3D) microstructured catalytic substrate was designed, and simulations of the fluid flow, heat transfer, and chemical reaction for the proposed catalytic substrates were performed using computational fluid dynamics (CFD) analysis. The effect of the pressure drop on the catalytic conversion efficiency of various 3D microarchitectures was investigated. Due to the three-dimensional microstructure, the fluid flow changed and fluid pressure increased, which led to energy loss. It was confirmed that the abrupt change in flow increased the heat transfer. The findings showed that the fluid flow changed due to the existence of a complex periodic microlattice structure instead of the existing monolithic structure, which promoted the conversion of harmful substances. Based on the CFD analysis of the thermal and fluid properties, it was confirmed that 3D microarchitectures can provide alternatives to conventional catalytic supports structures for efficient catalytic converters.

Keywords: microlattice; 3D microstructures; CFD simulation; pressure drop; thermal response; catalytic reaction

1. Introduction

Environmental pollution and diseases caused by harmful emissions from vehicles (such as CO, NOx, and HC) are on the rise; thus, countries worldwide are rapidly imposing restrictions relating to harmful components in exhaust gases [1]. To satisfy the strict regulations, studies are being extensively conducted on catalytic converters, which are representative devices for the reduction in hazardous emissions. In addition, many studies have focused on cold-start as an important issue that needs to be addressed to satisfy the regulations [2–4], as most of the harmful components in the exhaust gases emitted by automobiles are generated during cold-start [5]. The conversion efficiency of a catalytic converter is highly dependent on the temperature and the substrate’s thermal response [6]. Most conventional catalytic converters have a low thermal response and do not quickly reach the light-off temperature, resulting in low conversion efficiency. This leads to cold-start issues and excessive harmful emissions. Many previous studies have attempted to improve the substrate structure as a solution to this problem. The size of the catalytic reactor in a catalytic converter can be an important parameter. Previous studies have achieved a lower thermal inertia of catalytic reactors using small catalytic reactors, resulting in faster response between critical start-up and loading steps, which are important in automotive applications [7]. Foam-based catalytic converters are being researched to address cold-start problems in automotive applications owing to their lower thermal inertia and better mass and heat transfer properties than traditional honeycomb structures [8,9]. The effect of
the hollowness of a metal foam and the heat transfer characteristics of a porous open-cell metal foam has been investigated by simulation [10,11]. Porosity plays an important role in the overall heat transfer performance; in this regard, the use of a metal foam can considerably improve heat transfer but causes higher pressure drops [12]. Porous substrates with thin walls and high cell densities have low thermal inertias, large surface areas, and low hydrodynamic resistances of the working fluid. These characteristics are useful for assessing the issue of cold-start and increasing the catalyst activation and conversion rates [13]. Although the fabrication of microstructures with thin walls and high cell densities is challenging, recent advances in additive manufacturing technologies with functional materials can provide materials with controllable porosities and microstructures that enable the effective control of the working fluids [14–16]. A microlattice structure can also be designed for thermal management. A periodic lattice structure typically offers better mechanical performance than any foam [17]. Microreactors are widely used in modern chemical engineering owing to their energy efficiency and excellent durability [18]. By utilizing porous penetrating structures such as FCC and SC structures, it is possible to induce an inertial flow and improve the mass transfer [19]. A high geometric surface area and low heat capacity are required in the design of the catalytic carrier to improve the performance of catalytic converter systems [20]. There is a scarcity of reports confirming the substitutability and performance of existing monolithic structures by application of a fine lattice structure to catalytic transducers. Extensive research focusing on the thermal and fluid behaviors of microlattice structures is needed to confirm their potential as catalytic converters. To maximize the efficiency of catalytic converters, it is necessary to introduce a microlattice structure with a smaller volume and a larger surface area. In this study, catalytic converters were designed by introducing various three-dimensional (3D) microstructures to overcome the performance limitations of the existing structures. The objective was to determine the pressure drop and thermal response of the catalyst substrates that have 3D microstructures with different surface areas and relative densities and to analyze their effect on the performance of a catalytic converter. Fluid flow, heat transfer, and chemical reaction computational fluid dynamics (CFD) simulations of the proposed catalytic structures were performed using the COMSOL Multiphysics software. Results of the thermal response and pressure drop for the various catalyst substrates were obtained. Based on the results, the analyzed structures were capable of overcoming the limitations of conventional catalytic converters and improving their performance.

2. Materials and Methods

2.1. Methods

As shown in Figure 1, the 3D microstructures have typical thin walls and high cell densities, which leads to lower heat capacities and larger surface areas than the monoliths widely used as substrates in conventional catalysts. Owing to this, they might overcome the limitations of conventional catalytic converters. To ensure an accurate thermal response comparison, it was considered that heat capacity was the main factor controlling the thermal response and that it was directly proportional to the volume of the substrate. Thus, a small-volume substrate has a small heat capacity. However, a small-volume substrate also corresponds to a reduced catalyst volume; thus, the surface area and reaction performance of the catalyst are reduced as well. The monolithic structure hinders heat transfer to the substrate due to the influence of the channel wall structure [21]. It is expected that the geometry of the 3D microstructure will be suitable for the flow, which will aid in more active heat transfer to the substrate. By analyzing the thermo-fluid behavior of various 3D microstructures, it is necessary to compare the effects of the monolith structure and 3D microstructure on the catalyst substrate and catalytic conversion performance.
The performance of a catalytic converter depends mainly on the temperature of the catalyst substrate, as it directly influences the reaction rates. However, the pressure drop through the catalytic converter is another important variable that must be considered when considering the efficiency of the vehicle. A large surface area is required for the efficient removal of hazardous emissions, but the substrates with high surface areas tend to increase the pressure drop through the catalytic converter, leading to power losses and fuel waste. Thus, the trade-off between the pressure drop and the total surface area is a major concern in determining the appropriate geometry of a catalytic converter [22–24].

2.2. Governing Equations

The governing equations for the changes in concentration through a chemical reaction, fluid flow, and heat transfer are detailed in this subsection [25].

Fluid flow

\[ \rho \frac{\partial u}{\partial t} + \rho (u \cdot \nabla) u = -\nabla p + \nabla : [\mu I + K] + F \] (1)

Here, \( \rho \) is the density of the fluid, \( u \) is the velocity vector, \( p \) is the pressure, \( I \) is the identity matrix, \( K \) is the viscous stress tensor, and \( F \) is the volume force vector.

Turbulence is a characteristic of flow fields and is characterized by a wide range of flow scales. The tendency of turbulence is measured by the Reynolds number. The Reynolds number depends on the fluid density and velocity, length scale, and dynamic viscosity. The Reynolds-averaged Navier–Stokes (RANS) equation shown above indicates that the pressure term and viscous stress term change as the velocity changes. As the velocity and dynamic viscosity of the fluid change, the Reynolds number changes, enabling analysis of the turbulent flow.

Heat transfer in fluid

\[ \rho C_p \left( \frac{\partial T}{\partial t} + u \cdot \nabla T \right) + \nabla \cdot (q + q_r) = \alpha_p T \left( \frac{\partial p}{\partial t} + u \cdot \nabla p \right) + \tau : \nabla u + Q \] (2)

Here, \( \rho \) is the fluid density, \( C_p \) is the fluid heat capacity at constant pressure, \( u \) is the fluid velocity vector, \( T \) is the absolute temperature, \( q \) is the heat flux by conduction, \( q_r \) is the heat flux by radiation, \( \alpha_p \) is the coefficient of thermal expansion, \( p \) is the pressure, \( \tau \) is the viscous stress tensor, and \( Q \) corresponds to all heat sources other than the viscous dissipation.

Temperature changes due to a change in the pressure and the kinetic energy due to viscosity is converted into thermal energy.
Heat transfer in the solid

\[ \rho C_p \left( \frac{dT}{dt} + u_{\text{trans}} \cdot \nabla T \right) + \nabla \cdot (q + q_r) = -\alpha T : \frac{dS}{dt} + Q \]  

(3)

Here, \( \rho \) is the solid density, \( C_p \) is the solid heat capacity at constant pressure, \( u_{\text{trans}} \) is the velocity vector of translational motion, \( T \) is the absolute temperature, \( q \) is the heat flux by conduction, \( q_r \) is the heat flux by radiation, \( \alpha \) is the coefficient of thermal expansion, \( S \) is the second Piola–Kirchhoff stress tensor, and \( Q \) is corresponds to all additional heat sources.

Chemical reaction

\[ r_j = k_j \prod_{i \in \text{react}} c_i^{-v_{ij}} \]  

(4)

Here, \( r_j \) is the reaction rate of reaction \( j \), \( k_j \) is the rate coefficient in reaction \( j \), \( c_i \) is the concentrations of species \( i \), and \( v_{ij} \) is the stoichiometric coefficient of species \( i \) in reaction \( j \).

The following Arrhenius expressions describe the temperature dependence of rate coefficient \( k \).

\[ k = A \exp \left( \frac{-E}{R_g T} \right) \]  

(5)

Here, \( A \) is the pre-exponential factor, including the frequency factor, \( E \) is the activation energy, and \( R_g \) is the gas constant.

\[ \nabla \cdot J_i + u \cdot \nabla c_i = R_i, \quad J_i = -D_i \nabla c_i \]  

(6)

Here, \( J_i \) is the mass flux diffusive flux vector, \( u \) is the mass-averaged velocity vector, and \( R_i \) is the reaction rate expression for species; \( D_i \) is the diffusion coefficient.

The mass flux relative to the mass-averaged velocity, \( J_i \), is used in the aforementioned mass balance equation, with boundary conditions and for flux computations. The second term on the left side of Equation (6) describes the convective transport due to a velocity field \( u \).

2.3. Modeling and Boundary Conditions

The substrate structures used for the simulations were the monolithic, Schwarz Primitive triply periodic minimal surface (P-TPMS), simple cubic (SC), Kelvin cell, and octet structures; the unit cells are shown in Figure 1. Monoliths are commonly used as conventional catalyst substrates, and the cubic, Kelvin, P-TPMS, and octet structures have been used as 3D microstructures in several studies [26–29]. The dimensions of each cell were 1.27 mm (width, \( W \)) \( \times \) 1.27 mm (length, \( L \)) \( \times \) 1.27 mm (height, \( H \)). The strut diameters of the Kelvin, octet, and SC structures, as well as the thickness of the monolith walls and P-TPMS, were 100 \( \mu \)m. The catalyst substrates were modeled as 3 \( \times \) 3 cell structures. The same converter dimensions and unit cell of 3 \( \times \) 3 were used for all structures to compare the effect of each structure’s surface area and relative density on the performance of the catalytic converter. The detailed physical properties of the model used in the numerical analysis are shown in Table 1.

Table 1. Physical characteristics of the used structures (simple cubic, SC; Schwarz Primitive triply periodic minimal surface, P-TPMS; width, \( W \); length, \( L \); height, \( H \)).

<table>
<thead>
<tr>
<th>3D Microstructure</th>
<th>Monolith</th>
<th>P-TPMS</th>
<th>SC</th>
<th>Kelvin</th>
<th>Octet</th>
</tr>
</thead>
<tbody>
<tr>
<td>Surface area (mm²) (SA)</td>
<td>228.7</td>
<td>206.6</td>
<td>47.2</td>
<td>90.9</td>
<td>173.3</td>
</tr>
<tr>
<td>Solid volume (mm³) (Vs)</td>
<td>8.6</td>
<td>10</td>
<td>0.94</td>
<td>2.2</td>
<td>4.3</td>
</tr>
<tr>
<td>Surface area/Solid volume (1/mm) (SAV)</td>
<td>26.6</td>
<td>20.7</td>
<td>50.2</td>
<td>41.3</td>
<td>40.3</td>
</tr>
<tr>
<td>Relative density (( \rho_r = V_s/(27WLH) ))</td>
<td>0.15</td>
<td>0.18</td>
<td>0.017</td>
<td>0.04</td>
<td>0.078</td>
</tr>
</tbody>
</table>
The numerical analysis software used was COMSOL Multiphysics (ALSOFT, Seoul, Korea), version 5.6. The computational domain is shown in Figure 2. It consists of a fluid section for fluid flow, with dimensions of 3.81 mm (BC) × 7.81 mm (CH) × 3.81 mm (EH), and a ceramic substrate section, with dimensions of 3.81 mm × 3.81 mm × 3.81 mm. At the inlet (ABCD), boundary conditions were set for the temperature, fluid velocity, and concentration of the harmful gas species. At the outlet (EFGH), boundary conditions for preventing the backflow were set. No-slip conditions and surface reactions were set for the reactions of NO reduction and CO oxidation [32,33] and the subsequent catalytic conversion.

![Catalyst substrates](attachment:image1.png)

Information about the mesh is shown in Figure 3. The size of the mesh element was specified by dividing it into a fluid area and a 3D microstructure area using the free tetrahedral function. This function was used to create an unstructured tetrahedron and mesh the remaining domains, boundaries, edges, and points in the unselected areas. A corner refinement function was used to reduce the element’s size in sharp corners.

![Figure 3. Representation of a free tetrahedral mesh applied to fluid and solid domains.](attachment:image2.png)
Before examining the catalyst’s conversion efficiency, the thermal response of each catalyst substrate was checked. Thermal flow analysis was performed by assuming time dependence. Air and alumina were used as the working fluid and substrate, respectively. The initial temperatures of the fluid and ceramic substrate regions were set to 300 K. As boundary conditions, the inlet temperature was fixed at 1200 K (considering the exhaust heat of the engine), and the fluid velocity at the inlet was sequentially set to 1, 2, 3, 4, and 5 m/s. The fluid flow was assumed to be incompressible and turbulent, and the k-ε turbulence model was used [30,31]. To determine the effect of the pressure drop through the catalytic converter on catalyst conversion efficiency, a steady-state was assumed. Additionally, for the pressure drop analysis, the inlet temperature was fixed at 1200 K and the concentrations of the chemical species (NO and CO) at the inlet were set to 100 mol/m$^3$. The activation energies for the reactions of NO reduction and CO oxidation [32,33] and the diffusion coefficients were adopted from previous studies [34–36]. The fluid velocity at the inlet was sequentially set to 1, 2, 3, 4, and 5 m/s. As the catalytic conversion efficiency is highly dependent on the exhaust gas temperature [37], an analysis was performed to evaluate such effects. For this, a steady-state was assumed. The boundary conditions at the inlet were a fluid velocity of 1 m/s, a concentration of chemical species (NO and CO) of 100 mol/m$^3$, and temperatures sequentially set to 300, 500, 700, 900, and 1100 K.

3. Results and Discussion

3.1. Pressure Drop

Figure 4a,b show the pressure drop results for the different substrate structures. The change in the pressure drop was studied by sequentially increasing the inlet’s flow velocity. The pressure drop increases significantly in the order of P-TPMS > octet > Kelvin > SC > monolith. The largest values of pressure drop, as well as the largest change rates with the fluid velocity, correspond to the P-TPMS structure. This is due to P-TPMS being a converging–diverging structure, which causes the flow to change rapidly. The sudden change in the flow causes a large pressure drop and leads to a loss of kinetic energy. For the P-TPMS structure, a velocity of 1 m/s results in a pressure drop of 51.4 Pa and an increase in the velocity to 5 m/s results in a pressure drop of 514.3 Pa; this corresponds to an increase in approximately 1000%. The octet structure has the second-largest pressure drop, showing a value of 45.7 Pa for a velocity of 1 m/s. The pressure drop increases by approximately 825% by increasing the velocity to 5 m/s. In the monolith and SC structures, the pressure drop is not significant even when fluid velocity is high. Additionally, the flow is in a laminar regime.

3.2. Velocity Distribution

Figure 4c,j show the velocity distributions for the different structures. The flow in the octet and P-TPMS structures is turbulent. Previous studies showed that the local heat transfer is improved due to the vortices generated in the turbulent flow [38]. The velocity distributions of the monolith, SC, and Kelvin structures show that the flow is in the laminar regime; thus, these structures do not have the discussed effect on the heat transfer. By contrast, the turbulent flow accelerates the thermal response and leads to improvements in the catalytic reaction owing to the large surface areas of the structures and the mixing of the fluid. Thus, the turbulent flows of the octet and P-TPMS structures have an enhancing effect on the catalytic conversion efficiency, despite the negative aspect of their high pressure drops. The front views in Figure 3 show that the streamlines are distributed better in the octet and P-TPMS structures than in the other structures. The flow is classified as turbulent based on the Reynolds number of 2300 [20]. Thus, the results confirmed that only octet, Kelvin, and P-TPMS structures caused turbulent flow, with the maximum Reynolds numbers for each structure being 2709, 2796, and 6857, respectively. Although the maximum Reynolds number for the Kelvin structure is larger than that of the octet structure, considering the results for the turbulent kinetic energy, the octet structure is approximately twice higher than the Kelvin structure. Among the 3D microstructures, the
turbulent kinetic energy of the P-TPMS structure is the highest, which is approximately ten-times higher than that of the monolithic structure. Comparing the monolithic structure and octet structure, the turbulent kinetic energy is approximately seven-times higher in the latter.

**Figure 4.** Characteristics of the fluid flow through the 3D microstructures. (a) Pressure drop as a function of the fluid velocity; (b) pressure drop as a function of the axial position; (c,d,g,h) velocity distributions for the different 3D microstructures; (e,f,i,j) front view of fluid flow distributions.

### 3.3. Thermal Response

Figure 5a shows the volume-average temperatures of the 3D microstructures as functions of time and velocity. The thermal response rates of all structures increase with velocity. The Kelvin structure exhibits the highest thermal response, and the order of the values is as follows: Kelvin > octet > SC > P-TPMS > monolith. However, when the velocity is 5 m/s, the octet structure shows a higher maximum temperature than the Kelvin structure. Considering the efficiency of the converter, the catalyst must reach the light-off temperature rapidly. The catalytic conversion results show that the light-off temperature was approximately 500 K, which all microstructures reach in less than 0.5 s. Thus, the thermal
The thermal response rate chosen for the comparison was defined as the change in temperature after 0.5 s, divided by 0.5 s.

(a)

![Graph showing thermal response rates for different structures.](image)

(b)

![Graph showing thermal response as a function of velocity.](image)

**Figure 5.** Thermal response comparison for the different 3D microstructures: (a) volume-average temperatures as functions of time and velocity; (b) thermal response rates as functions of the fluid velocity based on a 0.5 s time frame considering the light-off temperature.

Figure 5b shows that the Kelvin structure has the highest thermal response rate, followed by the octet structure. As velocity increases, the curve of the octet structure gradually approaches that of the Kelvin structure. Although the thermal response rates of all structures increase with the velocity, the largest growth rate corresponds to the octet structure. Additionally, the P-TPMS structure has a faster thermal response than the monolith, despite having a higher relative density and a smaller surface area. This is due to
the mixing effect of the turbulent flow (as shown in the velocity distribution), which leads to faster heat transfer for the P-TPMS structure.

3.4. Chemical Reactions

Figure 6a,c show the influence of the fluid velocity on the performance of the catalysts. In general, an increase in the inlet velocity leads to an increase in the pressure drop across the catalytic converter; at the same time, the catalyst conversion efficiency decreases. However, a structure with a large pressure drop does not imply a low catalytic conversion efficiency. Although the octet structure has a larger pressure drop than the SC structure, its catalytic conversion efficiency is higher, and the SC structure has the lowest catalytic efficiency among all structures. Although the monolith structure has a lower relative density and larger surface area than those of the P-TPMS structure, the catalytic conversion efficiency of the P-TPMS structure surpasses that of the monolith as velocity increases. The octet structure has the highest catalytic conversion efficiency values, followed by the Kelvin structure.

![Figure 6](image_url)

**Figure 6.** CO and NO catalytic conversion results: (a) CO conversion as a function of the exhaust gas velocity; (b) CO conversion as a function of the exhaust gas temperature; (c) NO conversion as a function of the exhaust gas velocity; (d) NO conversion as a function of the exhaust gas temperature.

Figure 6b,d show the influence of the fluid inlet temperature on the performance of the catalyst. According to the experimental results of Pazmino [39], which depend on the temperature of the inflowing exhaust gas, CO conversion is approximately 70%. The results of this study show that the CO conversion of the monolith structure is approximately 69% (Figure 5b). This confirms the reliability of the simulation. The octet structure exhibits the highest catalytic conversion efficiency, as previously mentioned. This is due to the large...
surface area and octet structure reaching the light-off temperature quickly due to the lower heat capacity than monolithic and P-TPMS structures. The flow of the octet structure aids in the heat transfer of the structure. This can enhance catalytic reactions. Additionally, the surface area of the octet structure is approximately double that of the Kelvin structure, while its thermal response rate is the second-highest and quite similar to that of the Kelvin structure. The SC structure shows the lowest catalytic conversion efficiency, mainly because the reactive region (the surface area) was too small.

4. Conclusions

In this study, 3D microstructures were used to overcome the performance limitations of conventional catalytic converters. Fluid flow, heat transfer, and chemical reactions in the proposed catalyst substrates were simulated using COMSOL Multiphysics® software. The main conclusions of this study are as follows:

(1) Pressure drop and thermal reaction rate are significant variables that affect the efficiency of the catalytic converter. Pressure drop affects the vehicle’s driving efficiency and, thus, overall vehicle efficiency. The pressure drop of the octet structure can be large depending on the flow rate, but catalytic conversion efficiency does not decrease owing to the turbulent flow mixing in the structure. These results can help save energy by assessing the problems that lead to energy loss.

(2) Considering the overall catalytic conversion efficiency and driving efficiency, it was concluded that the Kelvin structure is the most suitable for catalytic converters.

(3) Finally, to increase the efficiency of the catalyst, the applied structure should have a high thermal response rate and a large surface area. The SAV ratio should not be considered the only parameter when designing the catalyst substrate. The SC structure had the highest SAV ratio among the studied structures, but it showed the lowest catalytic conversion efficiency in simulations. The SC structure has an extremely low relative density in comparison with the other structures; consequently, its thermal response was rapid. However, its catalytic conversion efficiency was low because the total reactive surface area was small. Thus, although it is crucial to reach the light-off temperature rapidly, the surface area of the catalyst structure is the most important variable in terms of catalyst conversion efficiency.

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