

# Mixed Reality-based chemical reactor visualization

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**Abstract:** A multi-tubular reactor for butadiene synthesis was developed, visualized using Microsoft HoloLens2, and built to allow immersive human interaction. Fluid analysis is particularly important in reactor design, including heat generation, temperature distribution, and mole fraction of reactants and products. Flow analysis is mostly executed with CFD tools like OpenFOAM and ANSYS Fluent. Post-processing software visualizes the CFD findings. However, the post-processing software is focused on the engineer, which lacks user-friendliness for the user who actually builds the reactor [Matthias Berger and Verina Cristie, 2015]. Contemporary technologies like virtual reality and mixed reality were applied to improve this. Virtual reality is a technique that creates a virtual world in a three-dimensional digital environment that blocks out the actual world. Furthermore, mixed reality technology interacts with virtual things made in the real world, minimizing heterogeneity and creating a smart environment where reality and virtuality are united by maximizing immersion. So, using Unity3D, a gaming engine, a multi-tube reactor was created in virtual reality. Menus, selection windows, and buttons are also implemented in C# to facilitate interaction. This VR was then deployed to Microsoft HoloLens2 via Visual Studio. The HoloLens2 is an untethered wearable holographic computer that offers bidirectional video, speech, and MR composite communication [Guy Martin et al., 2019]. An integrated mixed reality system was finally created that instantly reflected mutual conversation. This approach can also be employed in distillation towers, heat exchangers, separators, pumps and other process equipment performance monitoring. Smart manufacturing and a digital twin termed future plant can be accomplished by observing the actual process and implementing an autonomous data interaction system.

*Keywords:* Mixed Reality; Unity; HoloLens; Reactor; Visualization.

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## 1. INTRODUCTION

As a result of the significant improvements in computer-based and computer-aided engineering applications over the past decade (such as simulation, optimization, and monitoring systems) [Gbadago et al., 2020], some technological breakthroughs have occurred. The next phase of human-machine interaction, system monitoring, and digitization necessitates the employment of image rendering tools such as Unity3D, VR, and AR tools. Architectural designs [Fukuda et al., 2019], surgical procedures [Martin et al., 2020], mechanical applications, and staff training have all benefitted from using these instruments. Recently, a more advanced form of these technologies, known as the mixed reality [Zhu et al., 2020], is a next-generation information processing technology that enhances the usability and utility of information by mapping virtual generated information (e.g. Computer Graphic, Sound and Haptic, etc.) onto objects in a real environment in real-time for improved interactivity.

A smart environment in which reality and virtuality are integrated alleviates the heterogeneity and low immersion of augmented realities, making virtual images a part of the actual world.

Chemical engineering applications such as reactor systems and complicated process equipment are rarely used despite their

widespread use in construction, industry, and medicine. However, it is impossible to overstate the value of this technology in improving chemical process knowledge through mixed reality-based deep process performance visualization. Hence, this study proposes a stepwise approach for deploying chemical engineering results in a mixed reality environment based on CFD simulations and Unity3D. The CFD-Unity3D-HoloLens2 technique suggested in this work was used to develop an interactive environment that bridges the gap between process performance and monitoring. Using a multitubular reactor system, the butadiene reaction process was used as the demonstration study. Salome®, an open-source CAD program, was used to create the reactor, which had 14 tubes and a casing (see Fig. 1). Also, this mesh was also produced using the mesher function of the same software. Tetrahedral meshes were the most often created. Detailed information about the geometry's dimensions is shown in table 1. It was then transformed into an OpenFOAM-friendly mesh for CFD simulation. OpenFOAM is a CFD tool that uses the cell-centered finite volume approach. For example, the simulation was used to calculate the concentrations of oxygen, carbon dioxide, and butadiene. Target output variables were also thought to be temperature and velocity. Paraview-VTK® was used to post-process the simulated reactor results.

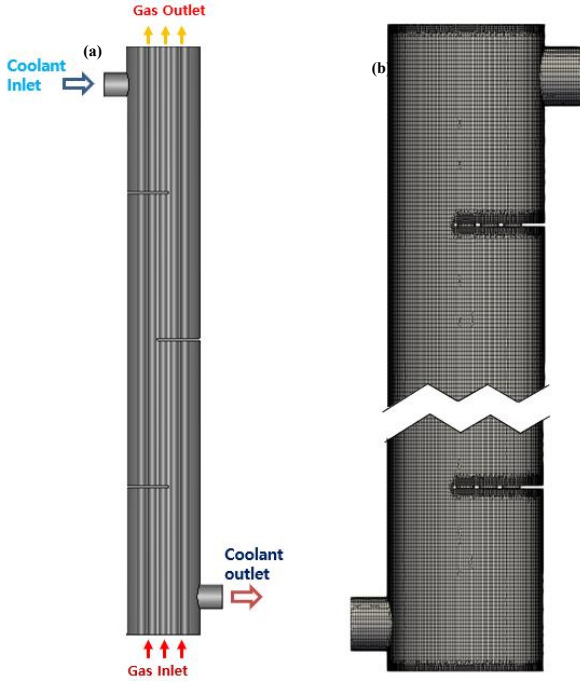


Fig. 1. Reactor modeling for CFD simulation (a) Geometry (b) Mesh

The reactor outputs must be translated into 3D picture formats before they can be rendered for 3D display. It has been suggested in the open literature that there are several 3D file formats that can be used. Each format has its own set of limitations, and the supported format varies depending on the software. For 3D file formats, glTF is one of the most versatile and lightweight options. For huge items like geometry, glTF has the ability to store them in a binary file, which can speed up the rendering process. As a result, the 3D images were rendered using the glTF 3D file format. A 3D engine called unity3D was used to further convert the rendered images into the virtual environment. A glTF reader was purchased in the Unity store to help render the glTF-generated 3D pictures with the correct texture. A panel was created to regulate the visual representation of the various elements. The completed product was converted into a format that could be used on a HoloLens2 by using mixed reality technologies. With the aid of the Microsoft visual studio program, the HoloLens2 (Fig. 2) was able to run the Unity3D® export file. Fig. 3 presents the overview of the strategy implemented here.



Fig. 2a. Microsoft HoloLens2

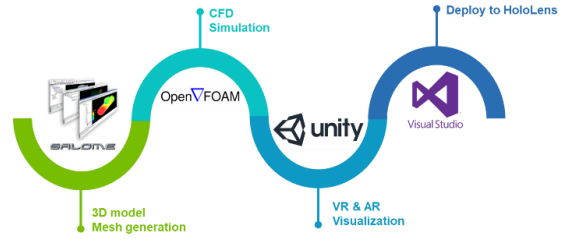


Fig. 2b. Different software employed throughout the study.

## 2. MATHEMATICAL MODELLING

This section elaborates on the mathematical modeling and conservation equations employed in executing the CFD simulations. The employed equations are presented (table 2)

Table 2. Equations for CFD simulation

Item	Equations
<i>Mass continuity</i>	$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = \dot{R}$
<i>Momentum Conservation</i>	$\frac{\partial}{\partial t} (\rho \bar{u}) + \nabla \cdot (\rho \bar{u} \bar{u}) = -\nabla p + \rho \bar{g} + \nabla \cdot (\tau + \tau_t) + \dot{R} \bar{u} + \bar{S}$
<i>Energy Conservation</i>	$\frac{\partial}{\partial t} (\rho h) + \nabla \cdot (\rho \bar{u} h) + \frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho \bar{u} k) - \frac{\partial p}{\partial t} = \rho \bar{u} \bar{g} + \nabla \cdot (\alpha_{eff} \nabla h) + \dot{Q}_{rxn}$
<i>Species Transport Equation</i>	$\varepsilon_p \frac{\partial}{\partial t} (\rho Y_i) + \varepsilon_p \nabla \cdot (\rho \bar{u} Y_i) - \varepsilon_p \nabla \cdot (\rho D_i \nabla Y_i) = (1 - \varepsilon_p) \rho_{cat} \dot{R}_i$
<i>Reactions</i>	$C_4H_8 + 0.5O_2 \xrightarrow{r_1} C_4H_6 + H_2O \quad \Delta H_r = -128.1 \text{ kJ / mol}$ $C_4H_8 + 6O_2 \xrightarrow{r_2} 4CO_2 + 4H_2O \quad \Delta H_r = -2552.6 \text{ kJ / mol}$ $C_4H_6 + 5.5O_2 \xrightarrow{r_3} 4CO_2 + 3H_2O \quad \Delta H_r = -2394.5 \text{ kJ / mol}$
<i>Reaction kinetics</i>	$r_1 = \frac{A_1 e^{-E_1/RT} P_B^n P_{O_2}}{(1 + K_{O_2} P_{O_2})(1 + K_B P_B + K_{BD} P_{BD})}$ $r_2 = \frac{A_2 e^{-E_2/RT} P_{O_2} (P_B - 3P_{BD})}{(1 + K_{O_2} P_{O_2})(K_B P_B + K_{BD} P_{BD})}$ $r_3 = \frac{A_3 e^{-E_3/RT} P_{O_2} P_{BD}}{(1 + K'_{O_2} P_{O_2})(P_B + P_{BD})}$
<i>Definitions of terms</i>	<p><math>\rho, v</math>, and <math>R</math> are the density, velocity, and mass source terms, respectively.</p> <p><math>\mu, g, R, p, S</math> are the dynamic viscosity, gravity, reaction source term, pressure, porous resistance in that order</p> <p><math>h</math> is the specific enthalpy, <math>k</math> is the turbulent kinetic energy, <math>Q_{rxn}</math> is the heat source due to chemical reactions, <math>\alpha_{eff}</math> is the effective thermal diffusivity (contribution of laminar and turbulent diffusivities).</p> <p><math>Y, D, R, \rho_{cat}</math>, are the mass fraction of species, the diffusivity, the species</p>

	reaction source term, and the catalyst density, respectively.
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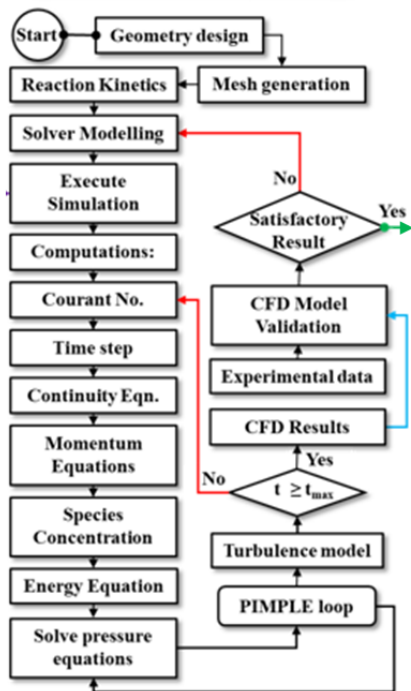
In this work, the oxidative dehydrogenation procedures utilized by Sterret et al. 1974 to convert butene to butadiene were used. Consequently, the temperature of the reaction zone is projected to rise as a result of the three processes. Previous research has detailed reaction parameters [Gbadago et al., 2020].

### Reactor modelling

- Geometry parameters  
Tube numbers, baffles, tube diameter, shell diameter, nozzle sizes, etc.
- Operating conditions  
Flowrate, temperature, compositions



### CFD simulation



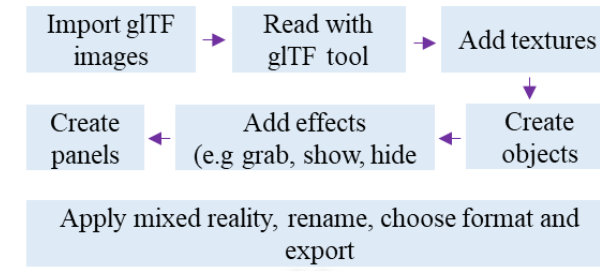
### Results postprocessing

#### PARAVIEW-VTK



### Mixed-reality environment

#### UNITY3D



### Deployment

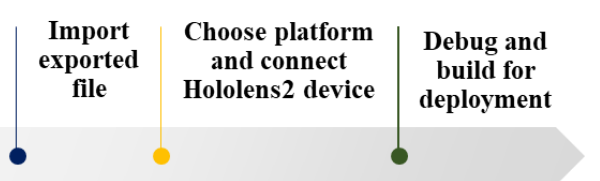


Fig. 3. The overall process of the proposed Mixed reality visualization strategy.

Table 1. Geometric design parameters of the reactor

	Shell	Tubes	Nozzles (Inlet/outlet)	Baffles	Tubes
D (m)	0.16	0.0254	0.05	Number (-) 3	Number (-) 14
L (m)	0.8128	0.8128	0.05	Spacing (m) 0.675	Pitch (m) 0.0083

## RESULTS AND DISCUSSION

The CFD simulation results and the created mixed-reality environment are shown here. Figure 4 shows some CFD results from a Paraview-VTK simulation. The temperature distribution in the shell and tube and the butene concentration profile were shown here. The results represent the exothermic oxidative dehydrogenation of butene to butadiene, key raw material for making tires and other polymer products. These contours can be exported as glTF 3D pictures for Unity3d® processing.

Fig.5a shows the intended panel for interacting with the mixed reality environment. Fig. 5b shows the

reactor projected onto a physical table in our lab. Fig. 5b shows the degree of mixed reality interaction between a user's environment and a virtual area. Fig. 6 shows the mixed reality assisted visualization outcomes as displayed on a television screen for larger audience participation. Finally, in Fig. 7, we showed the interactivity between the user and the virtual environment using features such as grab, enlarge, change orientation, etc, without compromising the image quality. Therefore, this strategy presents a much more advanced visualization experience than traditional process viewing.

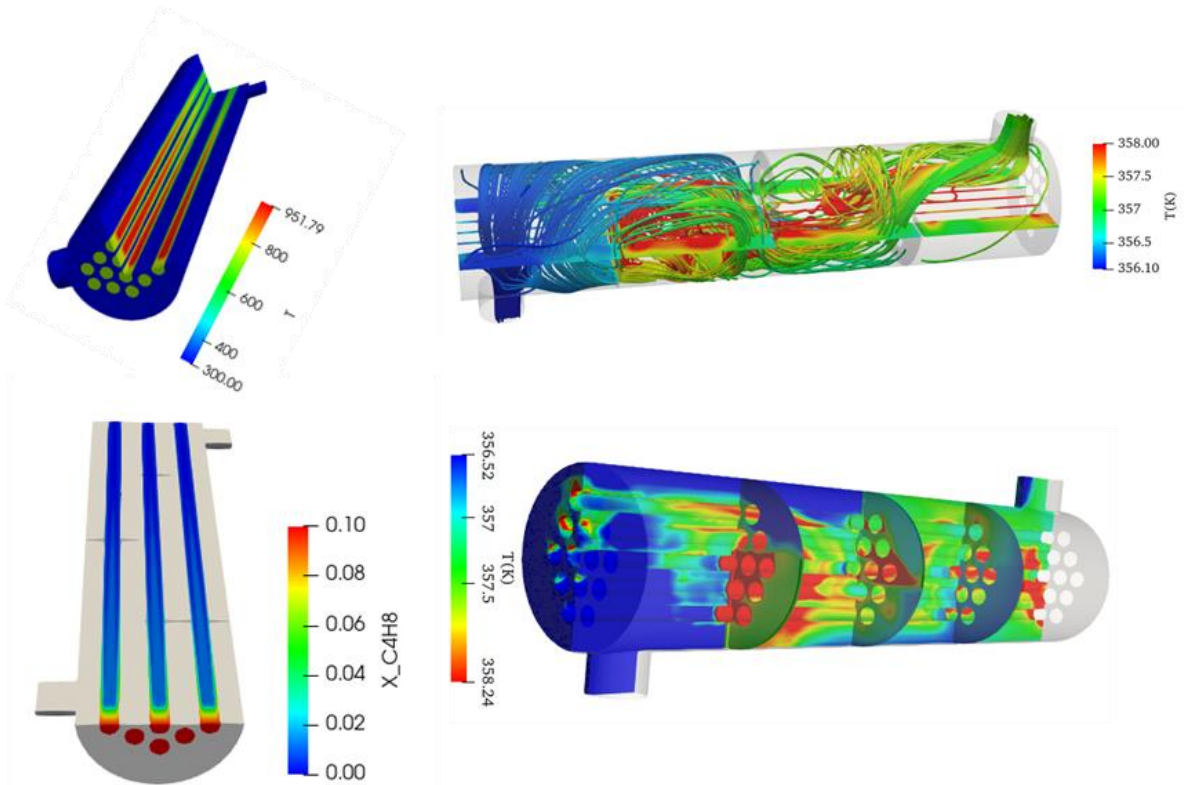


Fig. 4. Sample CFD results to be imported into glTF 3D image format

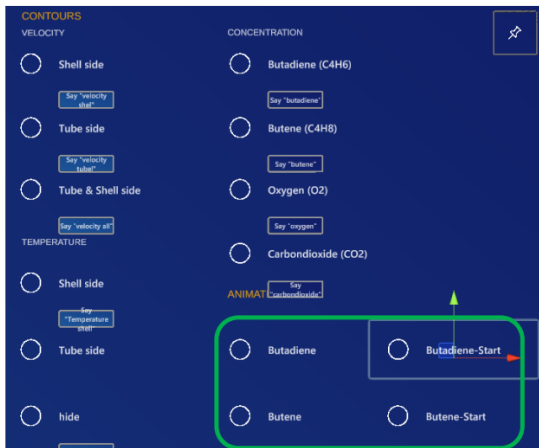


Fig. 5. (a) Interaction panel for mixed-reality experience, (b) Object projection into the mixed reality environment



Fig. 6. Projection of the virtual reality environment unto a TV screen for external audience visualization

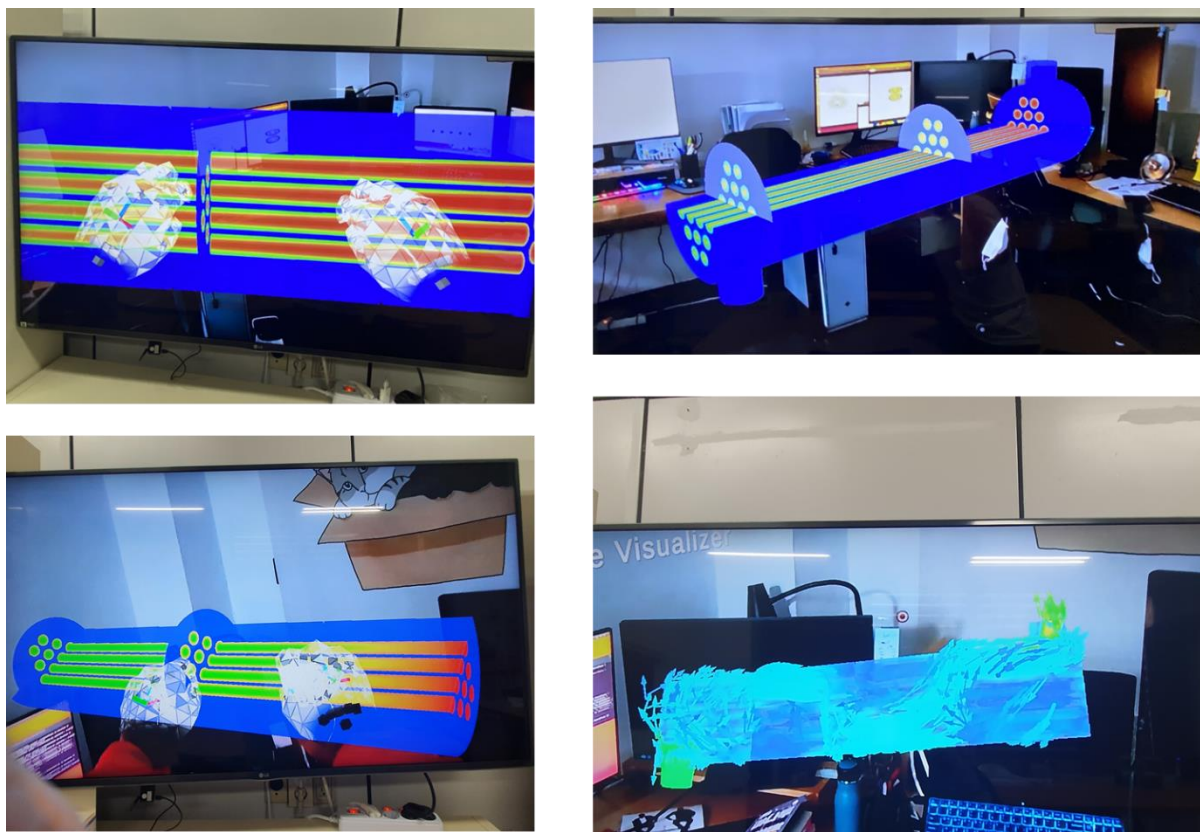


Fig. 7. Developed mixed reality environment for enhanced interactivity

### 3. CONCLUSION

We used CFD and CAD to construct an interactive reactor performance visualization technique in a mixed reality environment. The suggested approach can be applied to all types of process equipment for instructional purposes, deeper understanding of chemical systems, and more appreciative process behavior monitoring.

#### Acknowledgment

This research was supported by Korea Institute for Advancement of Technology(KIAT) grant funded by the Korea Government(MOTIE).(P0008475, Development Program for Smart Digital Engineering Specialist) This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (2019 R1F1A1058979)

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