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Optimization of the Vapor Flow Distribution in a Distillation Column Using Computational Fluid Dynamics

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Abstract

Chemical separations account for approximately half of the U.S.'s industrial energy use and 10-15% of the U.S.'s total energy consumption. More energy-efficiency chemical separation processes could save 100 million metric tons of CO_2 emissions annually. Specifically, distillation is the most widely used chemical separation technology, which accounts for approximately 40% of total energy consumption in petrochemical and chemical plants. Unfortunately, the overall efficiency is just around 11%. Therefore, it is necessary to improve the distillation efficiency, of which optimization of the spatio-temporal vapor distribution inside the column is essential. In this study, a computational fluid dynamics (CFD) model has been developed and employed to predict the vapor velocity distributions in a virtual 3-dimensional (3D) distillation column, with multiple inlet diameters (12 inches and 15 inches) and vapor flow rates (from 7929 lb/h to 27,750 lb/h) as the two key design parameters. The column height is approximately 8 feet, and the column diameter is 4 feet. Mellapak 250Y (M250Y) is used as the packing bed. Velocity contours and secondary flows at the top of the packed bed were compared to find the optimal design, with the minimum velocity variations across the plane. Coefficients of variation on the velocity distributions were also calculated and compared. Results indicate that with the increase of inlet Reynolds number, either due to the increase in inlet flow rate or the decrease in inlet diameter, the flow distributions become more uneven at the cross-section when the vapor flow exit the porous media region. Therefore, a low inlet Reynolds number is recommended for achieving a more evenly distributed vapor flow velocity.

Keywords: Distillation Column; Computational Fluid Dynamics (CFD); Porous Media; Velocity Distribution

Introduction

Chemical separations account for approximately half of the U.S.'s industrial energy use and 10-15% of the U.S.'s total energy consumption. More energy-efficiency chemical separation processes could save 100 million metric tons of CO_2 emissions annually. Specifically, distillation is the most widely used chemical separation technology, which accounts for approximately 40% of total energy consumption in petrochemical and chemical plants [2]. Unfortunately, the overall efficiency is just around 11%. Therefore, it is necessary to improve the distillation efficiency, of which optimization of the spatio-temporal vapor distribution inside the column is essential. However, experimental investigations are limited by the operational flexibility, locations for data sampling, and cost. It leads to unavoidable challenges to visualize and quantify the vapor transport phenomenon inside the column. As an alternative approach to overcome such limitations, computational fluid dynamics (CFD) based model has been introduced into the distillation process and design optimization [3]. For the distillation industry, CFD-based models discretize and numerically solve conservation laws of mass, momentum, and energy, with the capability to track spatial-temporal variations of variables inside the distillation columns. Furthermore, the CFD model can provide high-resolution predictions of the spatial-temporal variations for hydraulic and mass transfer inside the distillation column, which will provide a great amount of insight into the multiphase flow physics for the transitional and highly interactive process.

In this study, a CFD model has been developed and employed to predict the vapor velocity distributions in a virtual 3D distillation column (see Fig. 1), with multiple inlet diameters and vapor flow rates as the two key design parameters. Velocity contours and secondary flows at the top of the packed bed were compared to find the optimal design, with the minimum velocity variations across the plane.

Methodology

Geometry and Mesh

A virtual 3D distillation column was constructed based on a realistic design employed in industry (see Figure. 1). Specifically, the column height is approximately 8.534 m (8 feet), and the column diameter is 1.213 m (4 feet). The diameters (D_{in}) of the circular vapor inlet shown in Figure 1 are 0.305 m, and 0.381 m (12 and 15 inches in diameter). The center of the vapor inlet locates at (x,y,z)=(0,0,0), and the axial direction of the vapor inlet is aligned with the negative x-direction. The outlet diameter is 0.305 m (12 inches). The height of the Mellapak 250Y (M250Y) packing bed (see the blue region in Figure. 1) is 0.21 m, of which the porosity is 0.98. Polyhedron-based finite volume meshes with 10 near-wall prism layers were generated and mesh independence test was performed. As shown in Figure 1, the final meshes for the distillation column with different inlet diameters all contain approximately 300,000 cells, 1,000,000 nodes, and 1,500,000 faces.

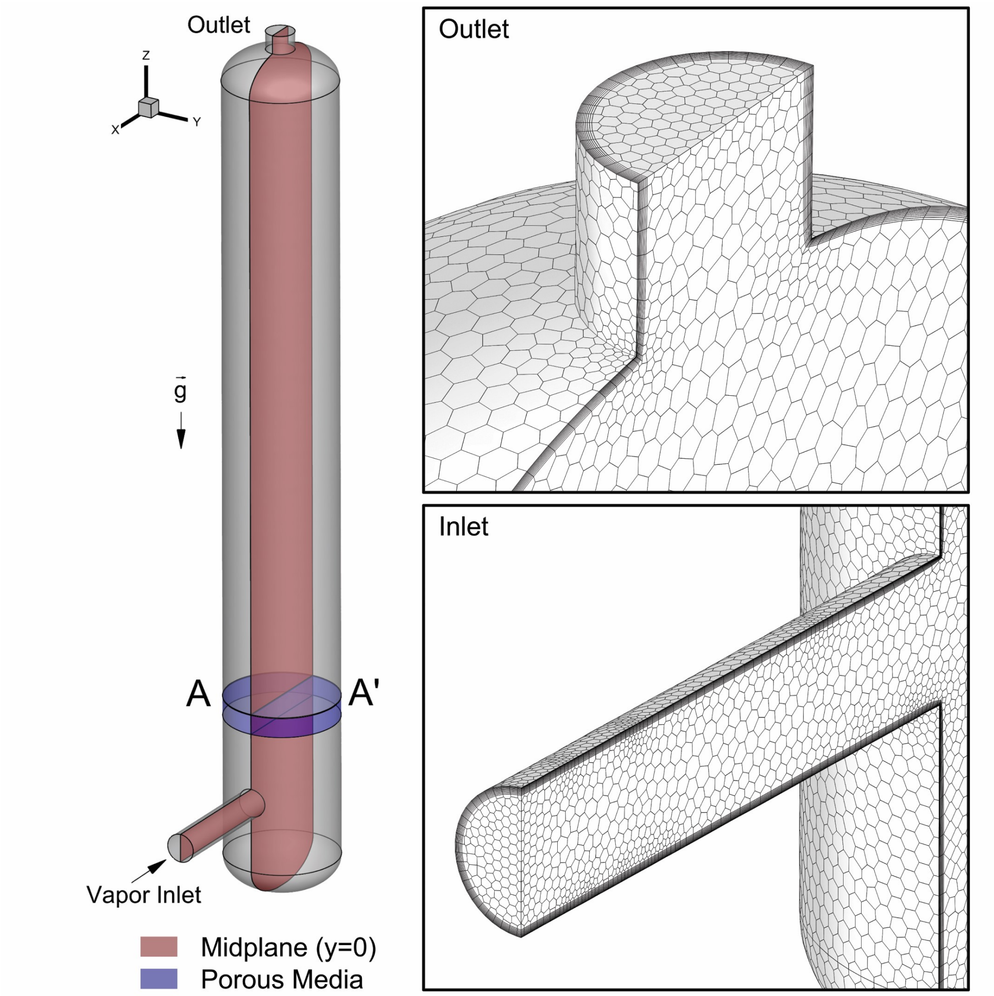

Figure 1: Examples of the geometry and mesh of a virtual 3D distillation column constructed (D_{in}=0.305 m)

Governing Equations

Conservation laws of mass and momentum were solved in this study. Specifically, the continuity momentum equations can be given as:

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (1)$$

$$\rho\left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right) = -\frac{\partial p}{\partial x_i} + \mu \frac{\partial^2 u_i}{\partial x_j^2} + \rho g_i + S_i \quad (2)$$

where u_i is the flow velocity, ρ is the vapor density, p is pressure, and g_i is the gravitational acceleration. In Eq. (2), the additional momentum source term S_i represents the bulk pressure loss through the packing bed, modeled as isotropic porous media. S_i can be given using the power-law model, i.e.,

$$S_i = -C_0\left(\sqrt{u_j u_j}\right)^{C_1} \quad (3)$$

where C_0 = 44.566 and C_1 = 2.0 in this study, representing Mellapak 250Y (M250Y) packing bed. Apparently, S_i =0 at the non-porous media flow domain inside the column.

To quantify the evenness of flow velocity distributions at the selected cross-section AA' (see Figure. 1), the coefficient of variation C_v of the velocity magnitude on 50 selected monitoring points on AA' were c calculated and compared. Specfically, the selected monitoring points are randomly distributed on AA'. C_v can be given as

$$C_v = \frac{\sqrt{\Sigma_{n=1}^{50}\left(\frac{U_n - \bar{U}}{\bar{U}}\right)^2}}{50} \quad (4)$$

where U_n is the velocity magnitude of monitoring point n, U is the average velocity magnitude of the 50 selected monitoring points.

Material Properties

Representing o/p-Xylene, the vapor density ρ is assumed to be 0.3844 kg/m^3 (0.024 lb/ft^3), vapor viscosity μ is 7.0e-6 kg/m-s (0.007cP).

Boundary Conditions

Vapor inlet mass flow rate m_{in} ranges from 1 kg/s to 3.5 kg/s (i.e., 7929 lb/h to 27,750 lb/h). Accordingly, a user-defined function (UDF) was employed to assign the fully developed tubular turbulent velocity profiles at the inlet, following the 1/7th power law [4]. Inlet Reynolds number (Re_{in}) ranges from 4.81e+5 to 2.10e+6. The outlet gauge pressure is assumed to be 0 Pa.

Numerical Setup

CFD simulations were performed using ANSYS Fluent 2021 R1 (ANSYS Inc., Canonsburg, PA) on a local Dell Precision T7910 workstation (Intel®Xeon® Processor E5-2683 v4 with dual processors, 32 cores, and 256 GB RAM), which took approximately 4 hours to finish one case. Some of the simulations were run on the supercomputer "Pete" at the High-Performance Computing Center (HPCC) at Oklahoma State University (OSU) (Intel®Xeon® Processor Gold 6130 CPU with dual processors, 32 cores, 64 threads, and 96 GB RAM). The Generalized k-ω (GEKO) turbulence model [5] has been employed to solve the turbulence flow field in the column. The SIMPLE scheme was selected for pressure-velocity coupling. Least squares cell-based scheme was selected for gradient spatial discretization. Second-order schemes were selected for spatial discretizations on pressure, momentum, turbulent kinetic energy, and specific dissipation rate. Convergence is defined for continuity, momentum, and supplementary equations, when residuals are lower than 1.0e-4.

Results and Discussion

Packing Bed Effect on Vapor Flow Distribution

To investigate the packing bed influence on vapor flow distribution, two distillation column simulations with D_{in} = 0.305 m were simulated and compared with and without the presence of the porous media zone. As shown in Figure. 2, the presence of porous media will significantly enhance the evenness of flow velocity distributions in AA'. The streamlines and velocity distributions also show the inlet flow jets impact the column wall and form an impingement flow structure. The impingement flow structure led to the high-velocity area shown in the velocity contours at AA'. Therefore, reducing the impingement intensity will be potentially beneficial to achieve a more evenly distributed vapor flow at AA'.

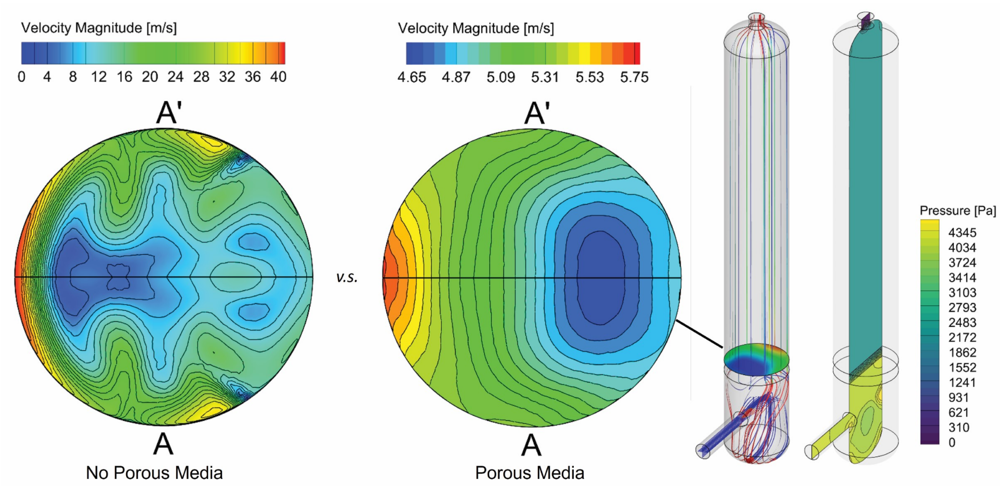

Figure 2: Comparison of velocity distributions at cross-section AA' for cases with and without porous media (packing bed) with m_{in}=2.256 kg/s.

Inlet Flow Rate Influence on Vapor Flow Distribution

Using a fixed inlet diameter (D_{in}=0.305 m) as a demonstration, 5 different inlet flow rates min=1, 1.5, 2.256, 3, and 3.5 kg/s. Comparisons of C_v and velocity contours at AA' are shown in Figure 3 (a)-(e). It can be found that with the increase in min, velocity distribution is more uneven due to the stronger impingement effect. Such an observation can also be proved by the increase in C_v with the increase in m_{in}

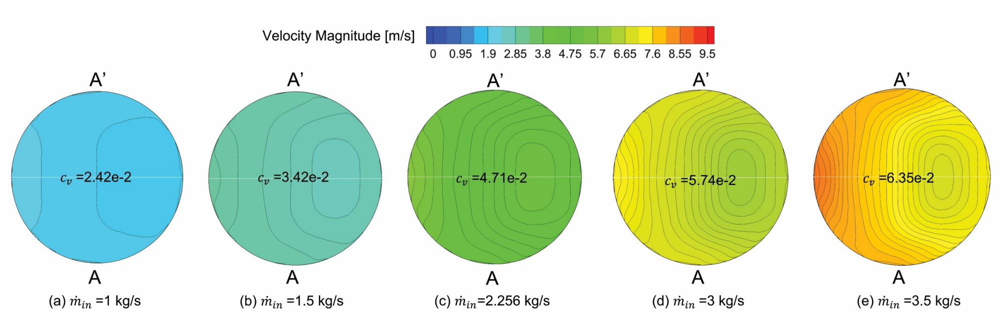

Figure 3: Comparisons of velocity contours and coefficients of variation at cross-section AA' for distillation column simulations with D_{in}=0.305 m: (a) m_{in}=1 kg/s, (b) m_{in}=1.5 kg/s, (c) m_{in}=2.256 kg/s, (d) m_{in}=3 kg/s, and (e) m_{in}= 3.5 kg/s

Inlet Diameter Effect on Vapor Flow Distribution

As mentioned in the previous section, columns with three inlet diameters (i.e., D_{in} =0.305 m and 0.381 m) were selected to investigate how inlet diameter can influence the vapor flow distribution. Figure 4 compares the coefficients of variation C_v with different inlet diameters and flow rates. At the same inlet flow rates, Figure 4 proves that with the increase in diameter, C_v decreases which indicates more evenly distributed vapor flow velocity.

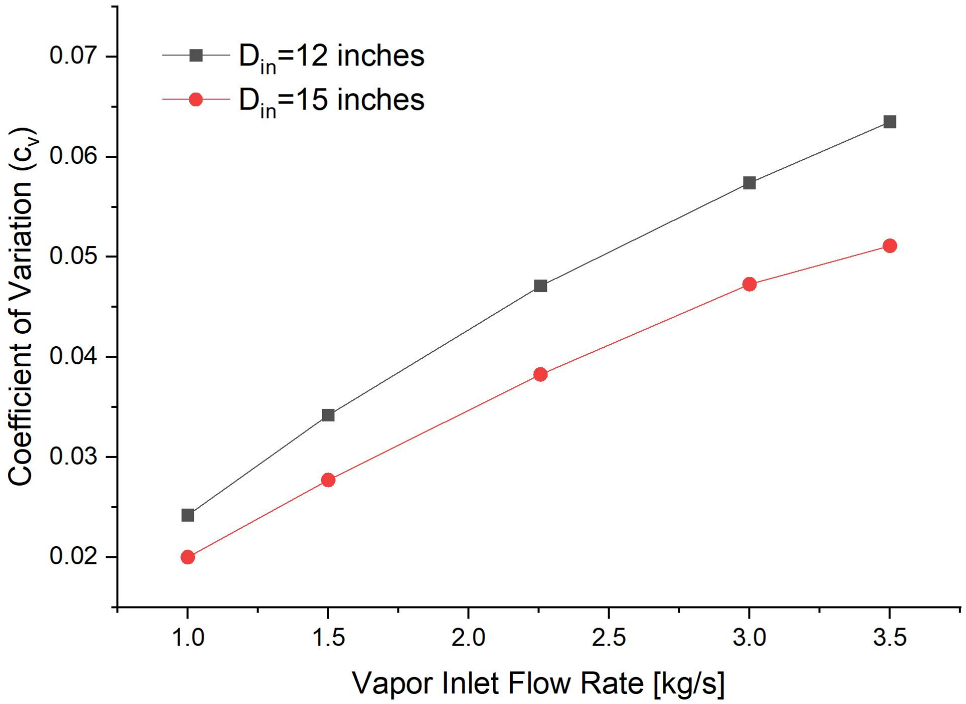

Figure 4: Comparisons of coefficients of variation with different inlet diameters and flow rates.

Influence of Re_{in} on Vapor Flow Distribution

Figure 5 plots the coefficient of variation C_v as a function of inlet Reynolds number Re_{in}. It shows that Re_{in} is a key factor that can impact the vapor flow distribution. Specifically, with the increase in Re_{in}, C_v increases in a quasi-linear pattern, despite the changes in inlet diameter D_{in}.

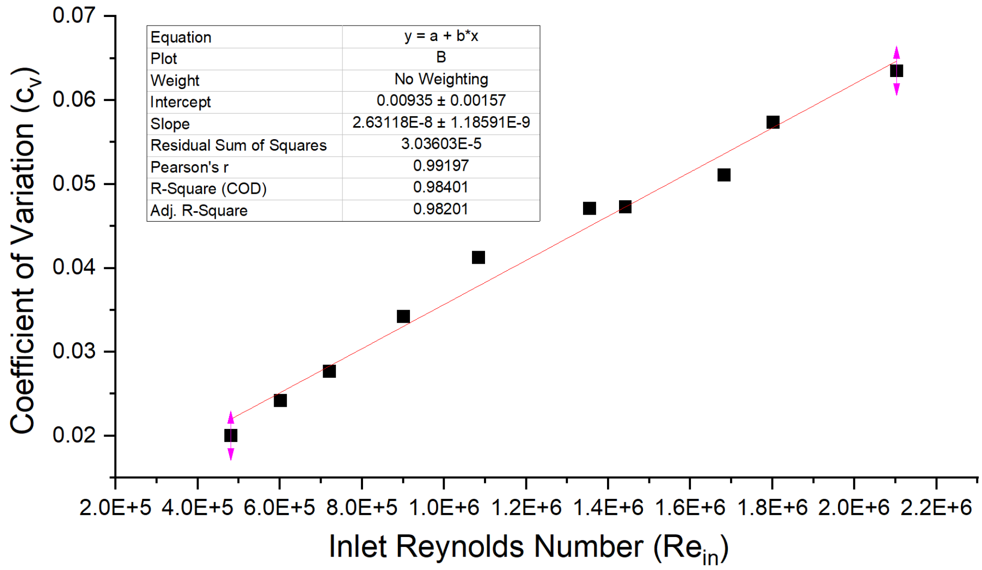

Figure 5: Relationship between the coefficient of variation C_v and inlet Reynolds number Re_{in}

Conclusions

A CFD-based model was developed and employed to investigate how porous media presence, inlet diameter, and inlet flow rates can influence the vapor flow distributions. It has been proved that with the increase of inlet Reynolds number, either due to the increase in inlet flow rate or the decrease in inlet diameter, the flow distributions become more uneven at the cross-section when the vapor flow exit the porous media region. Therefore, a low inlet Reynolds number is recommended for achieving a more evenly distributed vapor flow velocity.

Future Work

More simulations will be run with other combinations of design parameters. The CFD data, i.e., the C_v values labeled by the design and operational parameter values (inlet Reynolds number, and ratio between inlet and column diameters) will be employed as the training and testing data for a machine learning (ML) algorithm development, which will be used to characterize the optimal design of a distillation column.

Acknowledgment

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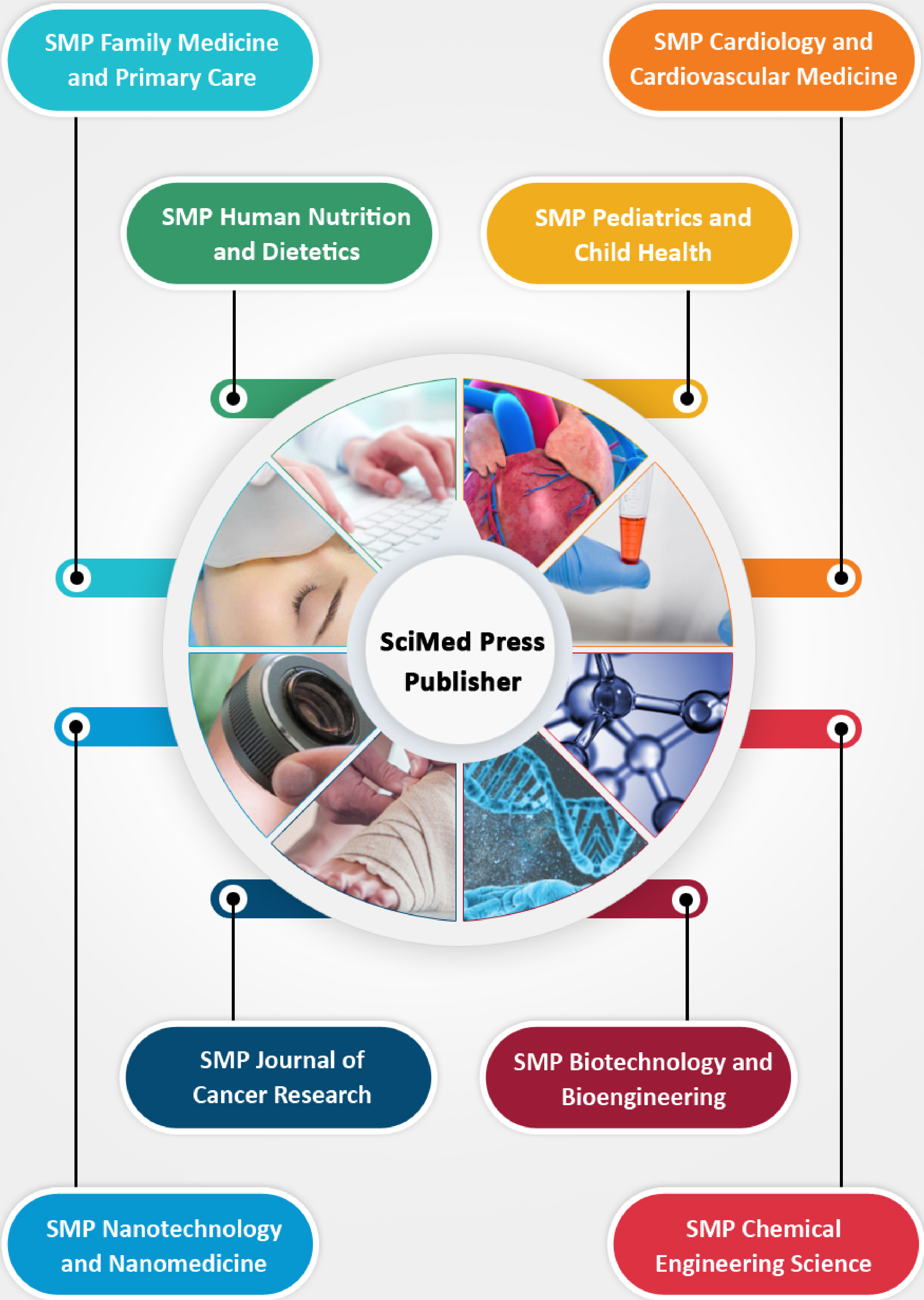
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