Mesh Sensitivity Analysis of 3-Dimensional Microchannel for Hydrodynamics Simulation of One Step Urea Synthesis

Reza Nurrahman, Anis Suhaila Shuib, Mohd Zamri Abdullah, Ku Zilati Ku Shaari
Department of Chemical Engineering
Universiti Teknologi PETRONAS
Perak, Malaysia
reza.nurrahman@gmail.com, {anisuha, zamriab, kuzilati_kushaari}@petronas.com.my

Abstract— **Urea (NH_2CONH_2) as fertilizer is important for agriculture industry. Potential one step urea synthesis patent based on magnetically induced process can bypass ammonia step by reacting H_2, N_2, and CO_2 directly at ambient temperature and pressure. At current state, the design of microreactor for one step urea synthesis is not available. The fluid flow of the gases for ammonia synthesis is simulated using in Computational Fluid Dynamics (CFD) approach. This study addressed the gap by focusing on finding the optimum microchannel design for the microreactor by varying geometry design. Mesh sensitivity study is performed to ensure acceptable results. In the microchannel where the scale is between micrometer to nanometer, the mesh quality can be reached by varying number of nodes in every geometry design. Investigating mesh quality can be obtained by measuring element quality, using Richardson Extrapolation method and Grid Convergence Index. The accepted mesh quality of most the geometry design is between 900,000 and 1,300,000 elements.**

Keywords-Microchannel; **microreactor; mesh; Computational Fluid Dynamics; Richardson Extrapolation;**

INTRODUCTION

Urea is an important fertilizer in agricultural industry. Novel urea production via one step synthesis use magnetically induced process [1]. In this method ammonia synthesis was achieved at room temperature (28ºC) and ambient pressure. The ammonia yield is increased when catalyst is placed in permanent magnetic field. Yttrium iron garnet (YIG) and α-Fe_2O_3 have been introduced as new nanocatalyst for ammonia synthesis. Due to the scale of catalyst, synthesis in microreactor will be suitable [2].

Efficient micromixing in microreactor is a solution to achieve effective production and decrease the needs of energy. Practically, there are some constraints typically featured in straight microchannel configurations. Increasing microreactor length will increase the efficiency [3, 4], which in turn increase the pressure drop [4]. Long mixing channel requires more energy for gas to flow. Therefore, shorter channel with satisfactory mixing and pressure drop criteria will be ideal.

Computational Fluid Dynamic (CFD) is a tool that is able to predict the flow in the microreactor. CFD which is widely known for cost saving, timely, and academically accountable is a useful technique for numerical calculation to verify or predict the fluid dynamics model. In the solution of the CFD model equation, numerical calculation is mostly using finite difference, finite element or finite volumes method.

In this paper, the pressure drop across irregular geometry of microreactor channel is investigated using CFD approach. The pressure drop of four microreactor geometry with varying turning angle is sought. Investigating mesh quality is an important step to reach CFD simulation condition. Coarse mesh can affect the calculation accuracy, but very fine mesh can prolong the simulation. Mesh quality was investigated based on Grid Convergence Index (GCI). The pressure drop is the basis for finding optimum mesh for simulation condition. Richardson Extrapolation method is used.

METHODOLOGY

A. Computational Design of Microreactor

Urea is produced by reacting three gases at ambient temperature and pressure [1].

$$N_2 + 3H_2 + CO_2 \rightarrow NH_2COONH_4$$

$$NH_2COONH_4 \rightarrow H_2O + NH_2CONH_2$$

At this stage, the magnetic effect is not considered. The general microreactor geometry is shown in Fig. 1 where the angle, Θ is varied at 90°, 120°, 135° and 150°. H_2, N_2, and CO_2 are reacted in the microreactor with diameter, d = 5μm, length, l = 20mm and volume = 392,500μm^3. Varying angle is important to optimize scattered gases molecules [5].

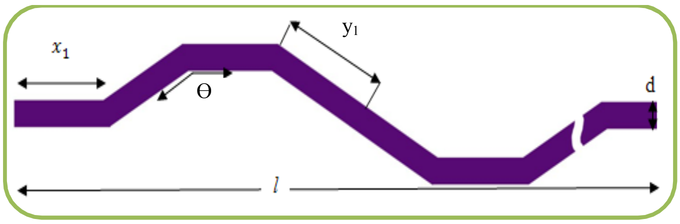

Fig. 1. Schematic of zig-zag geometry. d = 5 μm, l = 20 mm, x_1 = 1mm, and y_1 = |1/cos Θ| μm. Θ is varied at 90°, 120°, 135° and 150°.

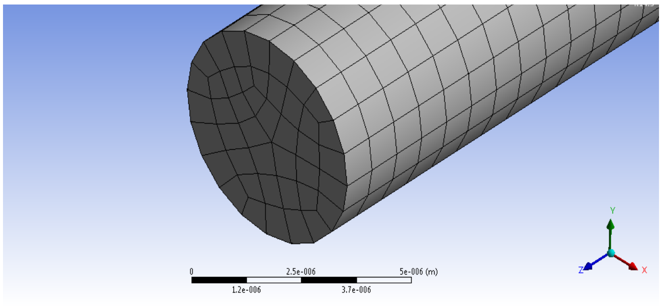

Fig. 2. Mesh at the inlet.

Four geometry were designed which are varied by turning angle of the microchannel. Varied geometry design are; Geometry 1 with 90°, Geometry 2 with 120°, Geometry 3 with 135° and Geometry 4 with 150°. After modeling four geometry designs, every geometry design was varied by number of elements. Varying number of elements aims at the optimum mesh for simulation condition, which the number of elements are varied from 60,000 – 1,300,000 elements, and number of elements of the stenosis geometry created was summarized in Table I.

TABLE I. NUMBER OF ELEMENTS, VOLUME SIZE OF ELEMENT AND TURNING ANGLE Θ

Turning angle of the microchannel, Θ.	**Number of Elements, N_i**	**Element density, μm^3/Element**
90°	N_1= 951,000	0.41
	N_2= 134,000	2.93
	N_3= 63,000	6.23
120°	N_1=1,040,000	0.38
	N_2= 576,000	0.68
	N_3= 130,000	3.02
135°	N_1=1,285,000	0.3
	N_2= 513,000	0.76
	N_3= 72,000	5.45
150°	N_1=1,110,000	0.35
	N_2= 513,000	0.77
	N_3= 171,000	2.30

ANSYS 14 was used to carry out each varied mesh in four geometry designs. The system is using laminar fluid flow in steady situation. Eulerian model in multiphase model in FLUENT was used to obtain three gases profile in the microchannel. In this model, the gases are not mixed and these gases only flow in a single microchannel. The aim of using eulerian model is only concerned by the pressure drop and elements. The governing equations for hydrodynamics process in microreactor are the conservation of mass given as:

$$\nabla.\left(\propto_q \rho_q \vec{v}_q\right) = 0 \qquad (1)$$

And the conservation of momentum given by:

$$\nabla.\left(\propto_q \rho_q \vec{v}_q\right)\vec{V}_q = -\propto_q \nabla \mathrm{p} + \nabla.\vec{\vec{\tau}}_q + \propto_q \rho_q \vec{g} \qquad (2)$$

Where q is the phase (H_2, N_2, or CO_2), $\vec{v}$ the velocity, α the volume fraction, ρ the density, p the pressure, and g is the gravity. The equation of shear stress tensor is given by:

$$\vec{\vec{\tau}}_q = \propto_q \mu_q\left(\nabla\vec{v}_q + \nabla\vec{v}_q^{T}\right) \qquad (3)$$

Where μ is the absolute viscosity.

The system boundary condition for H_2, N_2, and CO_2 velocity are 3.0859, 0.4373, and 0.2293 mm/s where the Reynolds number, Re = 1. Hence the model equation use is laminar flow where the wall material is aluminum which has roughness of 0.0015 mm and treated as having no slip condition. Pressure drop was calculated and compared between varied mesh.

B. Mesh Independence Study using Richardson Extrapolation Method and Grid Convergence Index.

Number of elements in the flow domain geometry determines the accuracy of the simulation. However, the smaller the number of elements the more computational effort is involved. Therefore, there had to be a balance between the size of the element volume and the computational cost, in order to yield accurate results. To resolve number of elements required, different mesh densities were tested to ensure that the flow solution is grid-independent. The solution criterion was the pressure drop across the microchannel. The pressure drop yielded by each mesh was analyzed to determine grid independence.

A stringent test is performed using Richardson extrapolation where the pressure drop value is estimated at the grid size tends to zero ($1/N \rightarrow 0$). In three-dimensional geometry, ratio of grid refinement, r can be replaced by ratio of control volume between fine and coarse mesh [6],

$$r_{12} = \left(\frac{N_1}{N_2}\right)^{\frac{1}{3}} \qquad (4)$$

The extrapolation method is a higher order estimate of the flow fields from a series of lower discrete pressure drop values. Roache generalized Richardson extrapolation by introducing the p-th order method [7],

$$f_{exact} = f_1 + \left[(f_1 - f_2)/(r_{12}^{p} - 1)\right] \qquad (5)$$

In this study, the function f_i (i = 1, 2, ..., n) referred to pressure drop across the microchannel, Δp_i [7]. *p-th* is the order of discretization method. Based on second order discretization, p is 2 for the system [6]. Then, pressure drop error can be obtained by:

$$Pressure\ drop\ error_i(\%) = \frac{|\Delta p_{exact} - \Delta p_i|}{\Delta p_{exact}}\ x\ 100\% \qquad (6)$$

GCI is based upon a grid refinement error estimator. It is computed using three grid sizes in order to estimate the order of convergence [8]. The relative error (ε_{ij}) is the measure of the function *f* between fine and coarse solutions,

$$\varepsilon_{12} = \frac{f_2 - f_1}{f_1} \quad (7)$$

The GCI for fine grid is defined by [8] as:

$$GCI^{fine} = \frac{F_S|\varepsilon|r^{p_R}}{(r^{p_R} - 1)} \quad (8)$$

Where F_S is a safety factor of 1.25. To verify if the predicted result is at asymptotic range, the α is defined as :

$$\alpha = \frac{r_{12}^{p} GCI_{12}^{fine}}{GCI_{23}^{fine}} \quad (9)$$

The solutions are in the asymptotic range of convergence, if the α is approximately one.

C. *Assessment of Mesh Quality*

In ANSYS 14, some tools are provided to be parameters to assess mesh quality for a whole body of geometry. The quality of mesh can be analyzed by cell quality parameter. This has significant effect on accuracy of numerical solution which consists of orthogonal quality, aspect ratio and skewness. These three parameters were calculated automatically by the software [9].

Orthogonal quality of each cell is calculated using the vector from centroid of cell to each of its face *i*. There are two equations for calculating orthogonal quality as follows:

$$\frac{\vec{A_i} + \vec{fc_i}}{|\vec{A_i}||\vec{fc_i}|} \quad (10)$$

$$\frac{\vec{A_i} + \vec{c_i}}{|\vec{A_i}||\vec{c_i}|} \quad (11)$$

Where $\vec{A_i}$ is the area vector, $\vec{fc_i}$ is the vector from cell centroid to the center of the face and $\vec{c_i}$ is the vector from cell centroid to the adjacent cell of shared face.

Skewness affects the accuracy and the stability. It is the difference between the shape of the cell and the shape of equivalent volume of an equilateral cell. Skewed mesh can be decided by skewness value within the range of 0 to 1.

The last parameter for mesh quality is the aspect ratio which measures the stretching of a cell. It is calculated as a ratio of the distance between the cell centroid and face centroid to the distance between the cell centroid and nodes. Orthogonal quality, skewness value and aspect ratio are calculated automatically by ANSYS 14 [9].

Results and Discussions

Mesh sensitivity and the pressure drop were analyzed.

A. *Mesh sensitivity analysis*

In mesh sensitivity analysis the accuracy of pressure drop across the whole geometry is analyzed. The results of pressure drop for four geometries are plotted in Fig. 3.

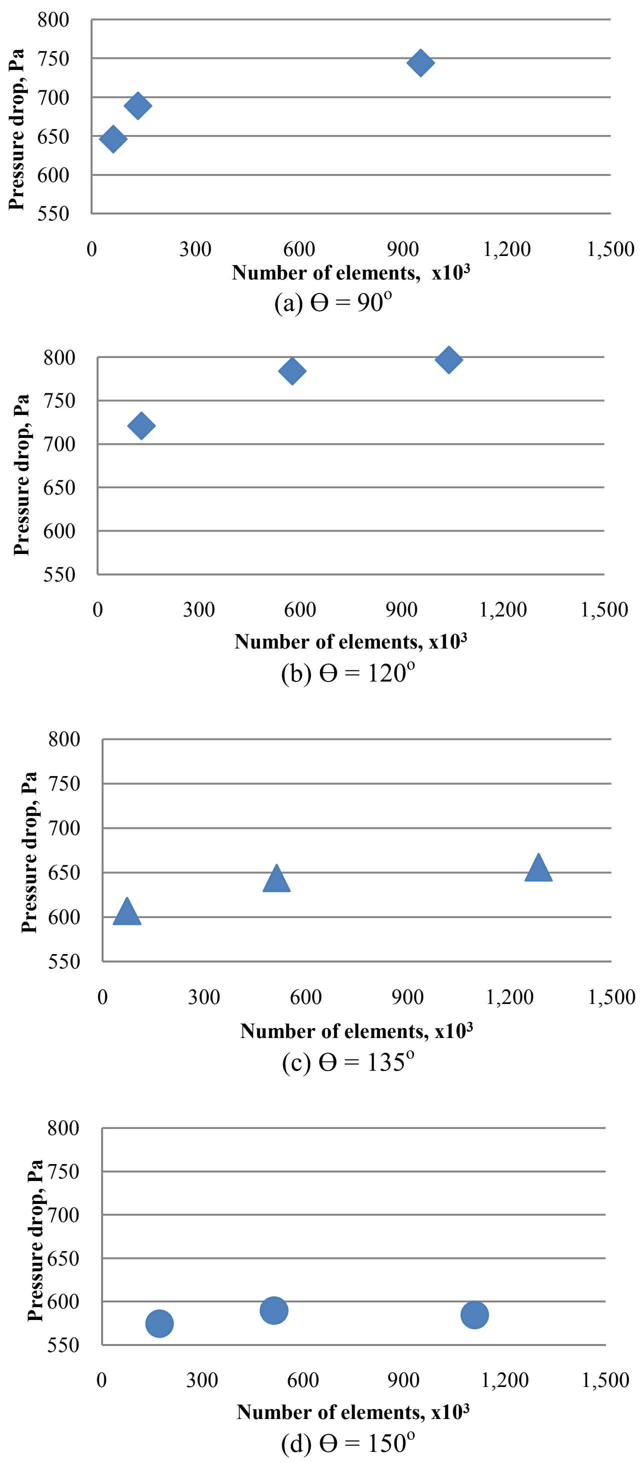

Fig. 3. Number of elements and pressure drop for (a) Θ = 90° (b) Θ = 120°, (c) Θ = 135°, and (d) Θ = 150°

The pressure drop is more consistent as the mesh further refined.

B. Relative Error and Grid Convergence Index Analysis

Data of relative error, GCI, and α of each turning angle is shown in Table II.

TABLE II. RELATIVE ERROR AND GRID CONVERGENCE INDEX

Turning angle of the microchannel, *θ*.	**Relative error, *ε*.**		**GCI**		**α**
	ε_{12}	ε_{23}	**GCI_{12}**	**GCI_{23}**	
90°	7.39%	3.43%	3.43%	11.93%	1.06
120°	1.63%	8.03%	4.22%	5.91%	1.05
135°	1.82%	6.03%	2.70%	4.55%	1.09
150°	0.85%	2.54%	1.58%	2.94%	0.90

It shows that ε_{12} and GCI_{12} for every turning angle are less than 5%, except θ of 90°. For hexagonal mesh, acceptable ε is reported less than 1□5% error margin [6, 10]. For turning angle 90°, it is more suitable to change to tetrahedral cell [9].

C. Determination of Exact Pressure Drop using Richardson Extrapolation Method.

The exact pressure drop is estimated using Richardson extrapolation method. Table III reported the data.

TABLE III. EXACT PRESSURE DROP DETERMINATION USING RICHARDSON EXTRAPOLATION METHOD

Turning angle of the microchannel, *θ*.	**Pressure drop across the channel, Δp_i (Pa).**	**Exact pressure drop using Richardson Extrapolation, p_R (Pa).**
90°	p1=646	p_R=764.4
	p2=689	
	p3=744	
120°	p1=721	p_R=823.92
	p2=784	
	p3=797	
135°	p1=607	p_R=670.21
	p2=644	
	p3=656	
150°	p1=575	p_R=577.57
	p2=590.42	
	p3=585	

From the data in Table III, the exact pressure drop was calculated. The exact pressure drop was predicted pressure drop when the mesh size is infinity.

D. Pressure Drop Error Assessment

The difference between simulated pressure drop at each mesh size and the exact pressure drop is determined. The error for each simulated pressure drop is presented in Fig. 4.

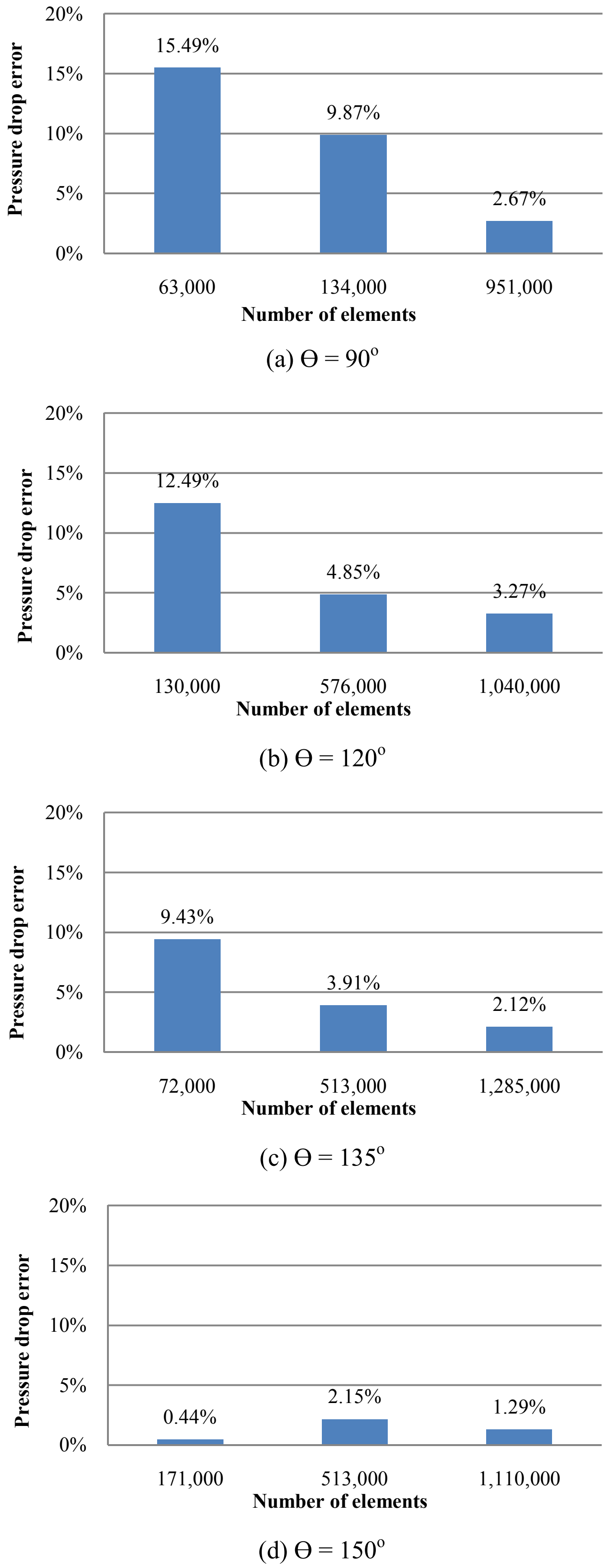

Fig. 4. Number of elements and pressure drop error for (a) Θ=90°, (b) Θ=120°, (c) Θ=135°, and (d) Θ=150°

The results obtained from percentage error are shown in Figure 4. From the data in Fig. 4, it is apparent that finest mesh that simulated in every turning angle can reach under 4% error. Acceptable margins of error reported were 5% error margin for categorical data and 3% for continuous data [11].

Every varied mesh was the finest mesh is chosen to represent the result in this simulation. Number of elements that has the lowest error for turning angle 90 ^{o}, 120^{o}, 135° and 150° are 951,000; 1,040,000; 1,285,000; and 1,110,000 elements, respectively.

E. Orthogonal Quality, Skewness and Aspect Ratio of Selected Mesh Geometry.

Quality of mesh is analyzed to focus on orthogonal mesh quality, skewness and aspect ratio. Table 4 is reported mesh quality for selected geometry.

TABLE IV. AVERAGE ORTHOGONAL MESH QUALITY, SKEWNESS AND ASPECT RATIO FOR SMALLEST ERROR GEOMETRY

Turning angle of the microchannel, θ.	**Mesh sensitivity error, %**	**Number of Elements**	**Average Orthogonal Mesh Quality**	**Skewness**	**Aspect Ratio (≈1.732)**
90°	2.67	951,000	0.72	0.45	1.75
120°	3.27	1,040,000	0.88	0.31	1.86
135°	2.12	1,285,000	0.92	0.26	1.91
150°	1.29	1,110,000	0.96	0.21	1.5

Value of orthogonal quality is between 0 to 1. The best cell has value of quality average (orthogonal quality) close to 1. Low skewness increases the accuracy and stabilizes the simulation solution. Value of skewness is between 0 and 1. The best cell has value of skewness close to 0. Aspect ratio measure the distance between the cell centroid and the face centroid. The best hexahedral cell has value of aspect ratio close to 1.732 [9].

Microreactor geometry with turning angle of 90^{o} has orthogonal quality value of 0.72, skewness of 0.45 and aspect ratio of 1.75. It represents the geometry has good quality mesh, but because of skewness value close to 0.5, the tetrahedral is more suitable than hexahedral cell [9].

Geometry with turning angle 120^{o} has orthogonal quality value of 0.88, skewness value of 0.31 and aspect ratio of 1.86. It is same case with geometry with turning angle 90 ^{o}. It is more suitable using tetrahedral mesh.

Both microreactors geometry with turning angle 135 and turning angle 150° have orthogonal quality value of above 0.9, skewness value of below 0.3, and aspect ratio close to 1.75. It represents the geometry has good quality mesh and can be operated in hexahedral cell.

CONCLUSIONS

The pressure drop decreases as the turning angle increase from 90 ^{o}, 120^{o}, 135^{o}, and 150^{o}. Steeper angle introduce greater of flow disturbance. Mesh quality of three-dimensional long microchannel for hydrodynamics simulation of fluid flow is investigated for turning angle of the microchannel 90 ^{o}, 120^{o}, 135^{o}, and 150^{o}. The mesh size with acceptable pressure drop errors across the microchannel are 951,000; 1,040,000; 1,285,000 and 1,110,000 elements, respectively. The mesh is selected for further simulation.

ACKNOWLEDGMENT

The authors would like to acknowledge funding from Ministry of Higher Education Malaysia under Long term Research Grant Scheme (LRGS) phase 1/2011.

REFERENCES

[1] Yahya, N., Puspitasari, P., Koziol, K., Asmawati, N., Fatih O.,M., Novel Electromagnetic – Microreactor Design for Ammonia Synthesis, International Journal of Basic & Applied Sciences IJBAS-IJENS 10, 1, 2011.

[2] Cao J. L., Wang, Y., Zhang T. Y., Wu S. H., and Yuan Z. Y., Preparation, characterization and catalytic behavior of nanostructured mesoporous CuO/Ce0.8Zr0.2O2 catalysts for low-temperature CO oxidation, Applied Catalysis B-Environmental, vol. 78, pp. 120-128, Jan 2008.

[3] Chen, C., Chang C. C., A combined active/ passive scheme for enhancing the mixing efficiency of microfluidic devices, Journal of Chemical Engineering Science 63,3081-3087, 2008.

[4] Jeon, W., Shin, CB, Design and simulation of passive mixing in microfluidic systems with geometric variations, Chemical Engineering Journal, 152, 575-582, 2009.

[5] Yi, M., Kim, D., Lee J., Koplik, J., Molecular Dynamics(MD) Simulation on the collision of a nano-sized particle onto another nano-sized particle adhered on a flat substrate, Journal of Aerosol Science 36, 1427-1443, 2005.

[6] Longest PW, Vinchurkar S., Effect of mesh style and grid convergence on particle deposition in bifurcating airway models with comparisons to experimental data. Medical Engineering Physics, 29, 350-366, 2007

[7] Roache, P. J., Quantification of Uncertainty In Computational Fluid Dynamics. Annu. Rev. Fluid Mech. 29, 123-160, 1997.

[8] Slater JW, Examining spatial (grid) convergence; 2008. <http://www.grc.nasa.gov/WWW/wind/valid/tutorial/spatconv.html>.

[9] Ansys. Inc. Release 14, 2011.

[10] Roy, C.J., Review of code and solution verification procedures for computational simulation, Journal of Computational Physics 205, 131-156, 2005.

[11] Krejcie, R. V., & Morgan, D. W., Determining sample size for research activities. Educational and Physichological Measurement, 30, 607-610, 1970.