ENHANCED ADVANCING FRONT TECHNIQUES FOR MESH GENERATION IN RADIATIVE HEAT TRANSFER PROBLEM

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To my husband, parents and family

– thank you for everything

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ABSTRACT

Mesh generation is a mathematical technique to produce meshes in the form of triangle and rectangles on a given domain for approximating values such as heat, temperature and pressure. The values are approximated using numerical methods such as finite element, finite difference and finite volume based on some given boundary conditions. In our work, a conceptual model has been designed for allowing a set of sensors to be deployed along the wall of an ethylene cracker furnace. The main function for the deployment is to provide input in the form of boundary values for approximating the temperatures of flue gas and the radiative heat flux distribution inside the furnace. New models called Enhanced Advancing Front Techniques (EAFT) have been proposed which improve on the existing standard advancing front in the form of element creation procedure, internal gradation control as well as the post-processing procedure for mesh quality improvement. EAFT is applied to discretise the domain of the conceptual model of the ethylene furnace with the requirements of having the location of sensors deployed along the wall as boundary nodes as well as forming boundary elements, generating nodes at a certain boundary with linearly different lengths of boundary edges using layer concept as interior gradation controls and constructing the triangular element directly in every iteration without having to re-order the front or delete the existing elements. The quality of the initial mesh is determined using the normalized measure of skewness provided by the GAMBIT software. The final mesh is obtained once the post-processing procedure of improving the mesh quality has been applied to the initial mesh. EAFT provides the framework for the heat to be approximated using the discrete ordinate method, which is a variant of the finite volume method. Simulation results produced using FLUENT support our findings for effectively approximating the flue gas temperature distribution, the circumferential radiative heat flux incident at the reactor coils as well as the circumferential reactor coil temperature in the conceptual model of ethylene furnace at the end of the study.

ABSTRAK

Generasi jaringan adalah satu teknik matematik untuk menghasilkan jejaring dalam bentuk segi tiga dan segi empat pada domain atau ruang tertentu bagi mendapatkan nilai anggaran seperti haba, suhu dan tekanan. Nilai anggaran didapati dengan menggunakan kaedah berangka seperti unsur terhingga, beza terhingga dan isipadu terhingga berdasarkan kepada beberapa syarat sempadan yang diberikan. Dalam kerja ini, model konsep telah direka untuk membolehkan satu set sensor yang akan digunakan di sepanjang dinding relau etilena. Fungsi utama sensor tersebut adalah untuk memberi input dalam bentuk nilai-nilai sempadan bagi mendapatkan nilai anggaran suhu gas serombong dan fluks sinaran haba di dalam relau. Model baru yang dipanggil *Enhanced Advancing Front Technique* (EAFT) telah dicadangkan untuk memperbaiki kaedah memajukan depan sedia ada dari segi prosedur penghasilan elemen, kawalan penggredan dalaman serta prosedur selepas pemprosesan untuk meningkatan kualiti jejaring. EAFT digunakan untuk membahagikan ruang model konsep relau etilena dengan memenuhi keperluan berikut; lokasi sensor yang di letakan di sepanjang dinding sebagai nod sempadan serta membentuk elemen sempadan, menjana nod di sempadan tertentu dengan jarak linear yang berbeza pada sempadan menggunakan konsep lapisan sebagai kawalan penggredan dalaman dan membina elemen segi tiga secara langsung dalam setiap lelaran tanpa menyusun semula depan atau memadam elemen-elemen yang sedia ada. Kualiti jejaring awal ditentukan dengan menggunakan ukuran kepencongan normal yang disediakan oleh perisian GAMBIT. Jejaring akhir diperolehi sebaik sahaja prosedur pemprosesan akhir untuk memperbaiki kualiti jejaring awal telah digunakan. EAFT menyediakan rangka kerja bagi menganggarkan suhu dan haba menggunakan kaedah ordinat diskret, yang merupakan varian kepada kaedah isipadu terhingga. Keputusan simulasi yang dihasilkan dengan menggunakan FLUENT menyokong penemuan kami untuk mendapatkan taburan suhu gas serombong, fluks haba sinaran pada lilitan gegelung reaktor serta suhu lilitan gegelung reaktor dalam model konsep relau etilena pada akhir kajian.

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LIST OF SYMBOLS / NOTATIONS

Roman Letters

a,b,c,d,e	-	nodes considered for element creation procedure
A, B, C, D	-	node forming the background grid
A_i	-	ith surface area
$b_{n,n+1}$	-	distance of the potential point from the edge which join node n and $n+1$
c	-	intersection with y-axis
d_i	-	layer
D_i	-	the product of the normal unit vector at the ith surface and the intensity direction Ω^m
E	-	emissive power
E_b	-	emissive power of blackbody
E_s	-	emissive power of real surface
$Edge\_sensor_i$	-	sensor boundary edge
i	-	node
i	dim -	dimensionality of the problem domain
IP	-	ideal point
K	-	number of pivot point
I	-	radiation intensity
I_b	-	radiation intensity of blackbody
I_s	-	radiation intensity of real surface
I^m	-	intensity along direction Ω^m

$I^{m'}$	-	intensity along direction $\mathbf{\Omega}^{m'}$
$I_{P_i}^{m}$	-	intensity at cell P_i
l	-	length of the selected shortest active edge
L	-	total length of the straight line
L_{bp1}	-	length between the connected node of the base edge and intersection point $p1$
Ld_i	-	Length of the layer
L_{base_edge}	-	length of the base edge
L_{ie}	-	the whole length of the intersected active edge
L_p	-	the length of the perpendicular line of the intersected active edge connecting directly to the IP
L_{p1p2}	-	length between the intersection points
m	-	number of layer
m_{ie}	-	the slope of intersected active edge
M	-	total number of discrete directions
M	-	number of sub-regions
n	-	node
n	-	total number of edges from the layer concept
n_s	-	number of nodes adjacent to node i
$\mathbf{n}$	-	outward surface normal
N_i	-	outer boundary nodes
p	-	centre of local umbrella
p	-	total number of inner boundary edges in the whole domain
p_s , p_e	-	point at local umbrella
$p1$, $p2$	-	intersection points of the active edge and circle
P_i	-	neighbour cell of cell P with ith surface as the same face between P and P_i
q	-	heat flux

q	-	total number of outer boundary edges in the whole domain
Q_{EAS}	-	EquiAngle Skew
Q_{EVS}	-	EquiSize Skew
r	-	radius of the circle for triangular element creation
r_j	-	reference number for inner boundary edge
r_k	-	reference number for outer boundary edge
r_l	-	reference number for edges from layer concept
r_t	-	reference number for new edge created in the whole domain
$\mathbf{r}$	-	position vector
$\mathbf{r_w}$	-	position vector for a point on a diffusively emitting and reflecting gray surface
N_n	-	optimal number of new points
N_P	-	total surface number for cell P
S	-	stretching parameter
S	-	area of the mesh elements
S_{eq}	-	maximum area of the equilateral triangle circumscribing radius of which is identical to that of the mesh element
T	-	absolute temperature
T_i	-	temperature obtained from the sensor at outer boundary node
$TEdge\_sensor_i$	-	average temperature value of sensor boundary edge
$w^{m'}$	-	solid angle associated with direction $\mathbf{\Omega}^{m'}$
x_j	-	x coordinate of the neighbouring node with reference number j
y_j	-	y coordinate of the neighbouring node with the reference number j
(x_a, y_a)	-	the co-ordinate of node a
(x_b, y_b)	-	the co-ordinate of node b

(x_c, y_c)	-	the co-ordinate of active node c
(h,k)	-	The co-ordinate of IP
(x_{p1}, y_{p1})	-	the co-ordinate of intersection point $p1$
(x_{p2}, y_{p2})	-	the co-ordinate of intersection point $p2$
(x_p, y_p)	-	the co-ordinate of the point where both of the perpendicular line and the intersected active edge cross

Greek Letters

α_n	-	angle between edges
δ	-	size parameter of the mesh
$\delta_{n-1,n}$, $\delta_{n,n+1}$	-	length of adjacent edge
ϕ	-	orientation of the cells
σ	-	Stefan-Boltzmann's constant
σ_s	-	scattering coefficient
ε	-	surface emissivity
κ	-	absorption coefficient
β	-	extinction coefficient
$\boldsymbol{\Omega}$	-	direction of intensity
$\Phi(\boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega})$	-	scattering phase function from the incoming direction, $\boldsymbol{\Omega}'$ to the outgoing direction, $\boldsymbol{\Omega}$
$\boldsymbol{\Omega}^+$	-	leaving radiation intensity direction
$\boldsymbol{\Omega}^-$	-	arriving radiation intensity directions
$\boldsymbol{\Omega}^m$	-	discrete direction of radiation intensity
μ	-	cosines of direction along the Cartesian co-ordinate x
η	-	cosines of direction along the Cartesian co-ordinate y

ξ	-	cosines of direction along the Cartesian co-ordinate z
ΔV_P	-	the volume of cell P
θ_{max}	-	maximum angle between edges
θ_{min}	-	minimum angle between edges
θ_{eq}	-	characteristic angle corresponding to an equilateral element

CHAPTER 1

INTRODUCTION

1.1 Research background

Ethylene is the greatest olefin market where most of it is consumed in plastic production [1]. 90% of ethylene in the Europe is produced from steam cracking using naphtha as the feedstocks while in North America and Middle East use ethane and propane as the feedstocks [2]. Ethylene is an important chemical compound produced in the petrochemical industry and is produced from the steam cracking process in ethylene cracker furnaces [3, 4]. In steam cracking, heat is used for breaking or cracking down the saturated hydrocarbon or feedstocks into smaller hydrocarbon in the reactor coils or reactor tubes, which eventually produces the desired products such as ethylene.

Of all the heat transfer modes, radiation plays a significant role in the ethylene production [5-10]. It has been noted in [6, 11] that more than 90% of the heat transfers in the ethylene furnace involve radiation. Radiation is caused by energy emission in the form of electromagnetic waves or streams of photons [12]. The heating process in the ethylene furnace begins when burners which are located on the floor near the furnace wall heat up the furnace. This happens because the combustion process carried out in the burner resulted in flames and the release of its hot flue gas. These flue gas are composed of carbon dioxide, water vapour, oxygen and nitrogen [13]. The radiative heat from the furnace wall and hot flue gas is then transferred to reactor tubes/coils.

The desired parameters of the heat transfer in ethylene furnace study are the temperature and the radiative heat flux. In order to obtain such parameters, the whole process of the fluid flow simulation in Computational Fluid Dynamics (CFD) need to be done where it involves all three elements namely pre-processing, solving and the post-processing. As a matter of fact, structured or unstructured triangular mesh formation fall into the pre-processing element in CFD [14]. The generation of triangular mesh is an important step for approximating solutions to boundary value problems. Among the two type of meshes, unstructured mesh are becoming predominant because of its ability of modeling complex geometry as well as the natural environment it has for adaptivity [15, 16].

There are two basic approaches for unstructured mesh namely the Delaunay triangulation and the advancing front technique. The Delaunay triangulation is a method of generating elements by adding or inserting points in the interior and reconnecting it to form the element [15, 17-21]. The insertion of the points can be controlled by several methods reported in [22]. On the other hand, the advancing front technique generate element with its key algorithmic step is the appropriate introduction of the new elements to the empty region [19, 21, 23]. It must be noted that the elements and the nodes in this technique are placed simultaneously in the region [24].

The advancing front technique places a new element by considering an ideal point generated as well as the existing nodes in the circle constructed. The centre of the circle is the ideal point and the radius is calculated based on the empirical rules for the element creation procedure. The advancing front technique is guaranteed to preserve boundary integrity as well as having the capacity to create triangular elements with high aspect ratios in the boundary-layer region [15, 25]. However, there are also method of combining the approach of Delaunay and advancing front techniques for generating unstructured mesh such as in [25-31].

In [32], the author highlighted three cases as being possible during the procedure of element creation with the approach of advancing front technique:

(1) A new element is created with a new node as a vertex in which the new node is joined to the edge being considered.
(2) An already existing front node satisfying certain conditions in the proximity of the edge being considered is used to create a new element.
(3) Neither of the cases above in which an efficient algorithm of mesh generation should be able to tackle such a problem.

With the advancing front technique as the approach for triangulation in the study, it can be seen that there is an improvement that need to be done towards the algorithm. The new improved algorithm of advancing front technique will be used to generate the unstructured meshes in the computational domain of the ethylene furnace for further modeling and simulation work.

1.2 Problem statement

The limitation of the current practice of monitoring and measuring the radiative heat transfer in ethylene furnace is addressed in this research. Furthermore, the current practice of the iterative approach in both finite volume and finite element also assume the initial intensity value to be zero because of unknown temperature distribution in the ethylene furnace. Hence, in this study a number of problems are addressed:

1) Given a set of sensors distributed along the wall of the ethylene furnace, in what way can the domain be partitioned into meshes in the form of triangle so as to support approximation of the temperature of the flue gas and the radiative heat flux distribution inside the furnace using methods like discrete ordinate, finite volume and etc?
2) What are the algorithms for effectively generating initial unstructured mesh that is appropriate for the conceptual model of integrating sensor network with the radiative heat transfer equation in ethylene furnace? The algorithm of the unstructured mesh must be able to tackle the problem of invalid or

undecided element creation in the algorithm.

3) What is the appropriate mesh post-processing procedure to improve the quality of the initial unstructured mesh if required?

1.3 Objectives and scope of the research

The objectives of the research are as follows:

Objective 1: To study the phenomena of heat transfer process in ethylene furnace and the current practice of monitoring the temperature and radiative heat flux.

Objective 2: To develop a conceptual model of integrating sensor network and radiative heat transfer equation in ethylene furnace.

Objective 3: To develop new algorithms for the initial unstructured grid that is appropriate for the conceptual model of integrating sensor network and radiative heat transfer equation in ethylene furnace.

Objective 4: To perform simulations using discrete ordinate method on the newly developed unstructured grid in order to obtain the smooth distribution of the flue gas temperature and radiative heat flux in the ethylene furnace.

The research concentrates on developing algorithm of initial unstructured triangular mesh for element creation procedure following the approach of advancing front technique in two dimensional domains. The research focused on triangular element since it is reported in [15, 16] that this element are the most flexible for complex two dimensional geometries especially when grading of the mesh is required. Although there are many more models in the ethylene furnace study, only radiation model will be considered for the present research. Therefore, the algorithm of unstructured mesh will be applied in the conceptual model of integrating sensor network and radiative heat transfer in order to obtain flue gas temperature and radiative heat flux in the ethylene furnace.

1.4 Research methodology

The methodologies in the research involve the following steps:

(1) Literature review

The ethylene furnace design, process descriptions, problem related to ethylene furnace, current techniques of modeling and simulating the ethylene furnace, the unstructured mesh formation and the discretisation technique as well as the type of temperature sensor will be studied through books, journal papers and conference proceedings. This first step is very helpful in order to obtain a wider view on the whole problem domain.

(2) Analysis phase

The furnace designs, the processes involved in the furnace as well as the selected problems are carefully analyzed. This is associated with the current methods and techniques of solving the furnace model with special attention to radiation model. At the same time, the basic concepts of advancing front techniques together with its recent approaches are analyzed for the conceptual model in the research. The analysis of the unstructured mesh is done through studying and applying the standard algorithm in both simple and complex computational domain in order to figure out any space for improvement. The current problems of undecided element creation are spotted when the algorithm of standard advancing front techniques are implemented in AutoCAD software to discretise several domains of the study.

(3) Design phase

A few versions of the algorithm of enhanced advancing front technique with a set of structured cases for element creation procedure are designed and developed to encounter the existing problem as stated in the last two paragraphs of Section 1.1. At the same time, the conceptual model of integrating sensors and unstructured mesh with radiative heat transfer equation in the furnace is designed. In the conceptual model, sensors are assumed to be placed along the wall of the furnace in order to

obtain boundary value for the radiative heat transfer model. The research focused on two dimensional model and therefore a cross section of the furnace is considered for the conceptual model.

(4) Implementation phase

As stated in Section 1.1, the CFD simulation involves three elements. The first element which is the pre-processing in this study involves the definition of the geometry of the ethylene furnace as the computational domain, mesh formation and the selection of physical phenomena that need to be modelled. In this study, the pre-processing element belongs to the implementation phase. The geometry of the ethylene furnace follows the one in the literature survey. The major contribution of the study focus on unstructured mesh, therefore, various simulation of the newly developed algorithm for the initial unstructured mesh is conducted and implemented in AutoCAD LT software. The selection of the physical phenomena of heat transfer as well as the fluid properties follows the existing research in ethylene furnace study.

(5) Testing and evaluation phase

As for testing and evaluation phase, the quality of the initial mesh implemented in the previous phase is determined using a number of measurements in GAMBIT 3.0 software. The mesh post-processing procedure is applied where required. The second element in CFD which is the solving process belongs to the testing and evaluation phase in the study. It involves numerical solution techniques using FLUENT software. As a matter of fact, this is one of the methods that can be considered to test and prove that the resulted unstructured mesh for the conceptual model is appropriate for further analysis. FLUENT is used to integrate and solves the governing equation of the heat transfer over all the unstructured mesh developed which represents the ethylene furnace. The discretisation technique of discrete ordinate method is used to convert the governing equation into a set of a system of algebraic equations. An iterative method is used to solve algebraic equations. The third element in CFD which is the post-processing also belongs to the testing and evaluation phase in the study. It involves the data visualisation for the final results. The results of the study are displayed as the contour of the flue gas temperature

distribution. Besides that, the circumferential radiative heat flux and the circumferential temperature of the reactor coils are also obtained and displayed in the study.

(6) Documentation

The work is reported in this thesis. The report presents all the concepts, simulation work, its analysis and results throughout the research.

The framework of the research is summarised in Figure 1.1a and Figure 1.1b.

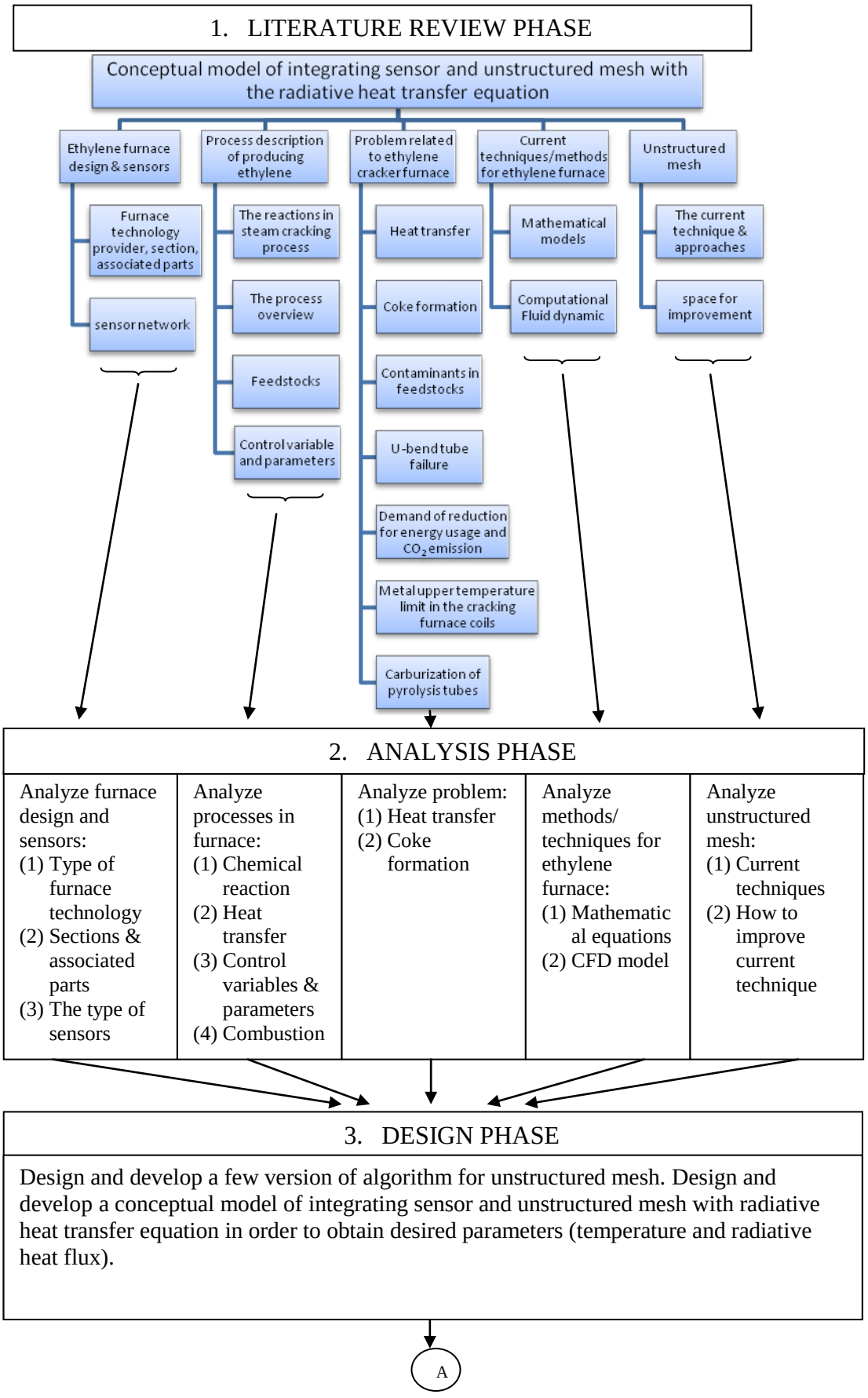

Figure 1.1a. The framework of the research – part 1.

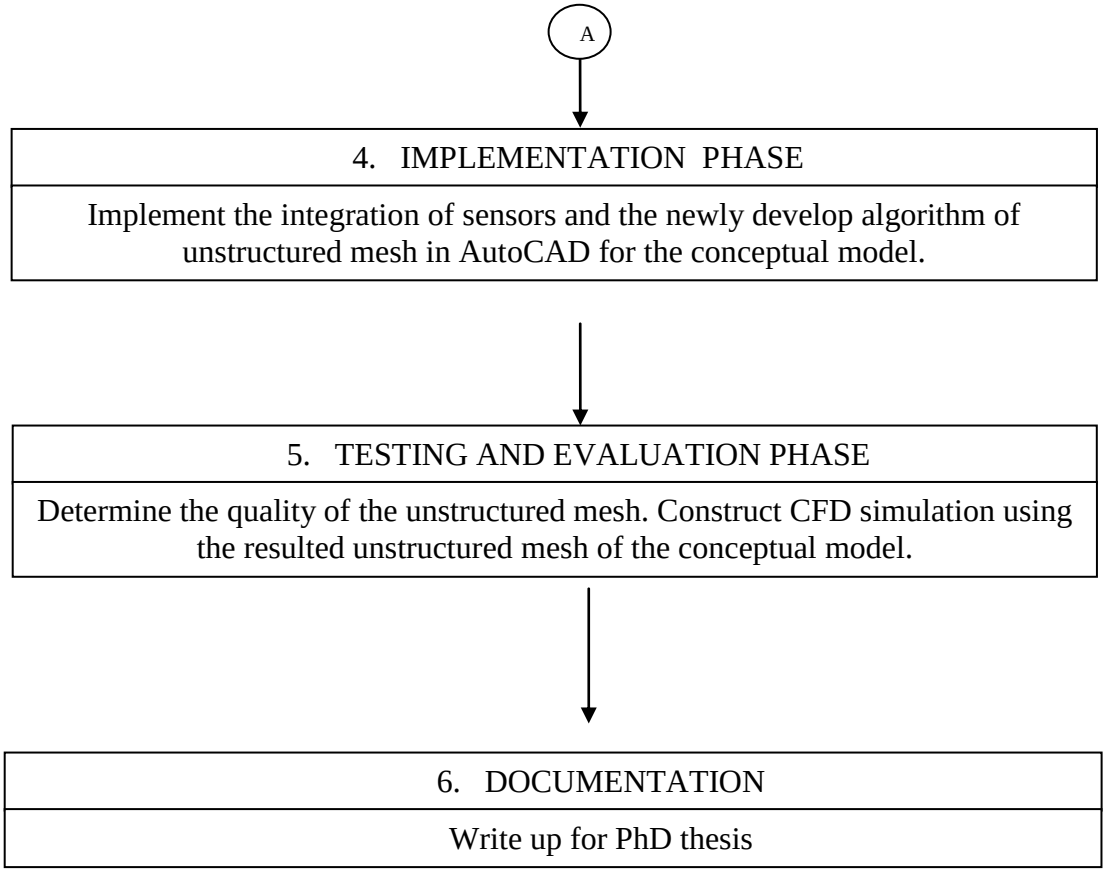

Figure 1.1b. The framework of the research – part 2.

1.5 Significance of the research

This research will contribute in improving the approach of modeling and simulation study in an ethylene furnace where most of the current techniques use only existing mesh generation software (GAMBIT etc) and CFD solver software (FLUENT, SPYRO etc) to predict the performance and behavior of operating parameters in the furnace operations. Since temperature plays a significant role in the daily operation of the ethylene furnace, it is of great importance to monitor the flue gas temperature distribution in the furnace, the radiative heat flux as well as the temperature of the reactor coils. This proactive approach of coupling a set of sensors in the furnace environment will provide continuous monitoring for further action to the furnace operator and engineers.

Therefore, a conceptual model of integrating sensor network and radiative heat transfer in the ethylene furnace environment is crucial as an initial phase of incorporating the ideas to the real world application. Sensors will be used to provide input in the form of boundary values for the simulation. Furthermore, the framework of the conceptual model provides the algorithm of initial triangular unstructured mesh where it incorporates the sensors deployment and a way of gradual mesh control. Besides that, it must be noted that the algorithm of the initial unstructured mesh is capable of constructing the triangular element directly in every iteration without having to re-order the front or delete the existing element as highlighted in the literature.

1.6 Outline of the thesis

An overview of the whole research is presented in Chapter 1 of the thesis. The research background of the ethylene furnace as well as the existing method of unstructured mesh formation is briefly described in the early part of the chapter. This is continued with the problem statements, the objectives and scope of the research as well as the research methodology and the significance of the research. The literature review is presented in Chapter 2 while a few versions of the unstructured mesh algorithm are developed and discussed from Chapter 3 through Chapter 5.

The discussion in Chapter 2 begins with an overview of ethylene furnace and its processes. This is followed by the phenomena of heat transfer in ethylene furnace and the current technique of monitoring heat transfer parameter where it serves as a foundation for setting up the conceptual model. The main contribution of the research is on the algorithm of unstructured mesh formation therefore an overview of related existing techniques of Delaunay mesh triangulation and advancing front techniques are discussed. This is followed by the existing mesh post-processing procedure for improving the quality of the mesh. The newly developed mesh is applied to solve the problem of radiation in the ethylene furnace, therefore the concept of radiation together with the Discrete Ordinate methods (DOM) as the

discretisation techniques are also described. At the end of the chapter, a review of the types of temperature sensors is presented.

Chapter 3 addressed the current problems in the element creation procedure of the standard advancing front technique. This problem has become a motivational reason of the need to enhance the current techniques in terms of element creation procedure. The first version of the newly developed algorithm for the unstructured mesh in this research is called as Enhanced Advancing Front Technique-1 (EAFT-1). The creation of the element in EAFT-1 is based on the five structured cases whereas the original technique has only two cases. The EAFT-1 is applied at a simple problem with enclosed wall where there is no inner boundary. The resulted unstructured mesh from the algorithm of EAFT-1 is integrated with the radiation model in order to proof that the mesh is appropriate for further analysis.

The second version of the unstructured mesh in Chapter 4 is called as Enhanced Advancing Front Technique-2 (EAFT-2). The element creation procedure in EAFT-2 is based on six structured cases. The radius of the circle during the element creation procedure does not follow the empirical rule as in SAFT but instead it is simpler than that. The departure zone for the element creation is set to be the entire front starting with the shortest edge. The algorithm of EAFT-2 incorporates the sensors as the boundary nodes forming boundary element. In order to tolerate the smaller size of element span over the shortest edges and the bigger size of the boundary element, the layer concept is introduced for internal gradation control of the mesh size. The EAFT-2 is applied at two simple conceptual models where in both conceptual model, the sensors are assumed to be placed along the wall. At the same time, the numbers of reactor coils in both simple conceptual models are reduced to only one complete reactor coil and half of the complete one reactor coil respectively.

The third version of the unstructured mesh in Chapter 5 is called as Enhanced Advancing Front Technique-3 (EAFT-3). The element creation procedure in EAFT-3 is based on seven structured cases. The radius of the circle during the element creation procedure in EAFT-3 is set to be eighty percent from the length of the base

edge. The departure zone for the element creation is set to be the specific front starting with the shortest edge. Similar to the approach introduced in Chapter 4, the layer concept is used for mesh size internal gradation control. A newly developed post-processing procedure to improve the quality of the mesh is also introduced in which it is called as EAFT-3 polygon refinement procedure. The algorithm of EAFT-3 is applied to the conceptual model which is designed and developed for ethylene furnace. The configuration of the ethylene furnace for the conceptual model followed the one in [33] and it is assumed that there is a set of sensors placed along the wall. The function of the sensors is to provide valuable input in the form of boundary value. At the end of the chapter, the resulted unstructured mesh incorporated with the conceptual model is applied for radiation problem in FLUENT software. The simulation converged and the desired parameters such as the flue gas temperature distribution, circumferential radiative heat flux and the circumferential skin temperature at the reactor coils are obtained.

The summary for every version of enhanced advancing front techniques can be found in Chapter 6. This final chapter also contains the contributions of the reearch in the aspect of unstructured mesh which are presented at the end of the chapter.

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