MULTIPHYSICAL MODELING AND OPTIMIZATION OF VACUUM BAG ONLY PROCESS WITH INTEGRATION OF RESIN FLOW, HEAT TRANSFER AND CONSOLIDATION FOR COMPOSITE MANUFACTURING DESIGN

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ABSTRACT

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Keywords: Prepreg, Process modelling, Out of Autoclave, Vacuum Bag Only, Multiphysics

The composite manufacturing for the aerospace industry requires advance and skillful manufacturing techniques. Autoclave manufacturing technique is well understood and widely used for the aerospace industry that aims to get as low as possible void content in cured parts with higher pressure and temperature profile. The allowable geometry of manufactured parts and operational cost limits Autoclave manufacturing techniques by fulfilling high mechanical performance. Alternatively, Out of Autoclave (OoA) technique with Vacuum Bag Only (VBO) method with right process conditions and prepreg system has the potential to displace expensive composite manufacturing challenges in the aerospace industry. The successful OoA manufacturing process depends on control of multiphysics such as resin flow, heat transfer and consolidation.

In this thesis, integration of multiphysical governing equations scheme for VBO manufacturing process, is developed and implemented for 2D through thickness of 1-, 2- and 4-layer of OoA prepregs via commercially available software. This model aims to capture instantaneous void content in prepreg system, hence, void initiation mechanism

and air evacuation channels during VBO process. The assessment of developed model during thesis, is planned to find time dependent change of resin impregnated area during VBO process. Based on change of resin impregnated area, the multiphysical assessment of developed model configurations is evaluated to reveal effective parameters of individual physics as well as integration with each other. The effective process parameters that includes initial cure temperature, post cure temperature, dwell time and ramp rate on the temperature profile is subjected to parametric numerical experiments as well as the optimization study with Nelder-Mead algorithm. The results of studies are aimed to find right process conditions in order to achieve repeatable, scalable and controllable VBO process outcomes.

ÖZET

KOMPOZİT ÜRETİM TASARIMINDA OTOKLAV DIŞI PREPREGLER İÇİN VAKUM TORBALAMA YÖNTEMİNİN REÇİNE AKIŞI, SICAKLIK TRANSFERİ VE KONSOLİDASYON ÇOKLU FİZİKLERİN ENTEGRASYONU İLE MODELLENMESİ VE OPTİMİZASYONU

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Anahtar Kelimeler: Prepreg, Proses modellemesi, Otoklav Dışı üretim, Vakum Torbalama, Çoklu fizik

Havacılık endüstrisi standardlarında kompozit üretimi ileri teknoloji ve yüksek kabiliyetli üretim teknikleri gerektirir. Otoklav üretim tekniği, yüksek basınç ve sıcaklık profili içeren, mümkün olduğunca düşük boşluk oranı elde etmeyi hedefleyen havacılık endüstrisi için iyi anlaşılmış ve yaygın olarak kullanılan bir yöntemdir. Üretilen parçaların kısıtlı geometrik özellklere sahip olabilmesi ve üretim maliyetlerinin cok yüksek olması Otoklav üretim tekniğinin kullanımını sınırladırmaktadır. Alternatif olarak, Otoklav Dışı (OoA) üretim tekniği ile Vakum Torbalama (VBO) yöntemi, doğru proses işlem koşulları ile havacılık endüstrisindeki pahalı kompozit üretim zorluklarının yerini alma potansiyeline sahiptir. Otoklav dışı vacuum torbalama yönteminin başarısı, reçine akışı, ısı transferi ve konsolidasyon gibi çoklu fiziklerin kontrolüne bağlıdır.

Bu tezde, VBO üretim süreci için çoklu fizik ana denklemleri şemasının entegrasyonu gerçekleştirilmiş ve 1-, 2- ve 4-katmanlı OoA prepreglerinin kalınlık yönünde iki boyutlu

(2D) çözüm geometrisi içerisinde, ticari olarak mevcut olan yazılım yardımıyla modellemesi gerçekleştirilmiştir. Bu geliştirilen model, prepreg sistemindeki anlık boşluk içeriğini, aynı zamanda boşluk oluşum mekanizmasını ve hava tahliye kanallarının tespit etmeyi amaçlamaktadır. Geliştirilen modelin tez içerisinde değerlendirilmesi, reçine emdirilmiş alanın VBO işlemi sırasında zamana bağlı değişimini bulacak şekilde ilerlenmiş. Geliştirilen model 1-,2- ve 4-tabakalı prepeg sistemleri için, hem entegrasyon hem de bireysel olarak herbir fiziğin değerlendirilmesi için kullanılmıştır. Sıcaklık profilinde ilk kür sıcaklığı, son kür sıcaklığı, bekleme süresi ve kürlenme hızı içeren etkili proses parametreleri, Nelder-Mead algoritması ile optimizasyon çalışmasının yanı sıra parametrik sayısal deneylere tabi tutulmuştur. Çalışmaların sonuçları, tekrarlanabilir, ölçeklenebilir ve kontrol edilebilir bir VBO proses çıktıları elde etmek için doğru proses koşullarını bulmayı amaçlamaktadır.

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ABSTRACT	IV
ÖZET	VI
ACKNOWLEDGEMENT	VIII
TABLE OF CONTENTS	IX
LIST OF TABLES	XII
LIST OF FIGURES	XIII
LIST OF SYMBOLS	XVI
Chapter 1	18
INTRODUCTION	18
1.1. Out of Autoclave Processes	18
1.2. Vacuum Bag Only (VBO) process	21
1.3. State of Art on Vacuum Bag Only Process Modelling	23
1.4. Scope and Organization of the Thesis Study	27
Chapter 2	
MODELING OF VACUUM BAG ONLY PROCESS	30
2.1. Vacuum Bag Only Process Modelling	30
2.2. Flow through Porous Media	33
2.3. Heat Transfer in Out of Autoclave Prepregs	
2.4. Consolidation in VBO process	
2.5. Equations of Empirical Relations	42
Chapter 3	45
NUMERICAL IMPLEMENTATION	45
3.1. Darcy Law	46
3.2. Flow Front Tracing Using Level Set Method	47
3.3. Heat Transfer in Prepregs	49
	-

TABLE OF CONTENTS

3.5. Consolidation with Arbitrary Lagrangian-Eularian Method (ALE)	52
3.6. The geometry of Solution Domain for OoA prepregs	53
3.7. Boundary and Initial Conditions	55
Chapter 4	50
OPTIMIZATION OF VACUUM BAG ONLY PROCESS	50
4.1. Problem Statement	51
4.2. Nelder-Mead Algorithm	52
4.2.1. Nelder-Mead Algorithm Implementation	54
4.2.2 Nelder-Mead Algorithm Case Study	56
4.3. Vacuum Bag Only process optimization for 1-Layer prepreg	58
Chapter 5	72
RESULTS AND DISCUSSION	72
5.1. Integrated Vacuum Bag Only Process Modeling Studies	72
5.1.1. Darcy's Law Adaptation	73
5.1.2. Darcy's Law coupled with Level Set Equation	76
5.1.3. Consolidation Physics with Arbitrary Lagrangian-Eularian Equation	78
5.1.4. Heat Transfer in Vacuum Bag Only coupled with Cure Kinetics an Viscosity Models	nd 81
5.1.5. Multiphysical VBO process modelling without consolidation	36
5.1.6. Void Analysis of 1-Layer Multi Physical Modelling of VBO process8	38
5.1.7. Void Analysis of 2-Layer Multi Physical Modelling of VBO process9) 1
4.1.8. Void Analysis of 4-Layer Multi Physical Modelling of VBO process9) 2
5.2. Integration Assessments for the void comparison	95
5.3. Parametric Study for the void comparison10	00
5.4. Optimization of VBO process10	04
5.4.1. Optimized Temperature Profile for 1- Layer)4
5.4.2. Optimized Temperature Profile for 2- Layer)7

Chapter 6	
SUMMARY, CONCLUSION AND FUTURE WORKS	
6.1. Summary and Conclusion	
6.2. Future Works	
REFERENCES	115

LIST OF TABLES

Table 3.1. Built in modules in COMSOL Multiphysics ®
Table 3.2.Coefficients of PDE equation in COMSOL Multiphysics ®
Table 4.1.Optimization types and options in COMSOL Multiphysics ®
Table 4.2. The initial temperature profile parameters used in this study
Table 4.3. The last values of the temperature profile parameters found with the Nelder-
Mead algorithm
Table 5.1. Material properties table for simple Darcy Law solution
Table 5.2. Defined parameters required to solve Level Set Equation
Table 5.3. Defined parameters required to solve Level Set Equation
Table 5.4. Thermal properties of resin and fiber for Heat Transfer equation
Table 5.5 The parameters used for the cure kinetics model
Table 5.6 The parameters used for the viscosity model
Table 5.7. Defined parameters for numerical simulations by physics
Table 5.8. Parameter ranges for numerical experiments 100
Table 5.9. The initial parameters used for the optimization studies104
Table 5.10. Optimized temperature profile parameters for 1 layer prepreg106
Table 5.11. Optimized temperature profile parameters for 2 layer prepreg

LIST OF FIGURES

Figure 1.1. Autoclave ovens used for the composite manufacturing [2],[3]
Figure 1.2. The schematic representation of Aerospace composite manufacturing
techniques and the place of Vacuum Bag Only process [4]20
Figure 1.3. Prepreg processing in Vacuum Bag Only process
Figure 1.4. VBO process steps with Out of Autoclave prepregs
Figure 1.5 The followed systematic for the development of multiphysical VBO process modeling
Figure 1.6.Pert chart of the thesis study
Figure 2.1.The defined and solved parameters in multiphysical modelling of VBO process
Figure 2.2. Schematic of permeability concept
Figure 2.3. Representative control volume of fluid for conservation equations during
impregnation of resin
Figure 2.4. The leading mechanism of VBO prepreg consolidation
Figure 2.5. Representation of air pore change during consolidation while impregnation
Figure 3.1. The representative section of level set parameter (ϕ) progression between two
fluids [39]
Figure 3.2. The name interpretation of main PDE equation
Figure 3.3. The goemtry determination procedure for KOM12 OoA prepregs, a) Light
Microscopy images, b) Micro-CT image, c) simplified geometry for modelling54
Figure 3.4. Boundary conditions for Darcy's Law56
Figure 3.5.Boundary condition for Level Set Equation to flow front tracking
Figure 3.6. General Heat Transfer boundary conditions
Figure 3.7. Consolidation physics boundary conditions
Figure 4.1. The optimization flow chart of developed model
Figure 4.2. The classical temperature profile during VBO manufacturing and the
representations of the optimization parameters on the temperature profile
Figure 4.3. The geometrical description of the Nelder-Mead algorithm [41]63
Figure 4.4. The flowchart of the integration of the model with the Nelder-Mead algorithm 64
Figure 4.5. Example problem flowchart for the Nelder-Mead algorithm

Figure 4.6. The time decided by the Nelder-Mead algorithm for this example problems
(left), the change of the objective function depending on the number of steps (right)68
Figure 4.7. The converging values of defined parameters in Nelder-Mead Algorithm71
Figure 4.8. Change of resin fill ratio with each iteration of Nelder-Mead algorithm
solution of 1-layer prepreg system71
Figure 5.1. Flowchart of integration of physics with Comsol Multiphysics®73
Figure 5.2. 2D Darcy Law boundary conditions74
Figure 5.3. 2D Darcy Law solution in example geometry for a) pressure distribution, b)
Darcy velocity distribution
Figure 5.4. The time dependent flow front positions for a fluid through porous media
under vacuum pressure
Figure 5.5. Time dependent consolidation effect on throught thickness of prepreg solved
with ALE79
Figure 5.6. The level set equation solution for the density Equation [3.3] as initial and
final solution time (0s-1000s)80
Figure 5.7. The level set equation solution for the viscosity Equation [3.4] as initial and
final solution time (0s-1000s)80
Figure 5.8. Recomended temperature profile for KOM-12 OoA prepreg system by
KORDSA®
Figure 5.9. The viscosity (blue) and the degree of cure (green) change during VBO
process
Figure 5.10. Exothermic heat generation (blue) graph during the degree of cure increasing
(green)
Figure 5.11. The cure rate dependent with degree of cure during process for used resin
system
Figure 5.12. The resin flow front evolution of multiphysical modelling of 1-layer of VBO
prepreg without consolidation physics
Figure 5.13. The resin flow front evolution of multiphysical modelling of 1-layer of VBO
prepreg with consolidation89
Figure 5.14. The comparison of resin impregnated area development during VBO process
for the models with90
Figure 5.15. The time dependent thickness change with regards to mesh movements
provided by ALE module for 1-layer VBO manufacturing process

Figure 5.16. The resin flow front evolution of multiphysical modelling of 2-layer of VBO
prepreg92
Figure 5.17. The resin flow front evolution of multiphysical modelling of 4-layer of VBO
prepreg94
Figure 5.18. Permeability change with respect to fiber volume fraction for 1, 2 and 4
layers prepregs durin the multiphysical VBO process modelling
Figure 5.19. Viscosity and degree of cure results for numerical experiments
Figure 5.20. Initial thickness change percentages for 1, 2 and 4 Layer
Figure 5.21. Void ratio results for initial cure temperature parameters101
Figure 5.22. Void ratio results for post cure temperature parameters102
Figure 5.23. Void ratio results for ramp rate parameters
Figure 5.24. Void ratio results for dwell time parameters103
Figure 5.25. Temperature profile parameters evolution in Nelder-Mead algorithm for 1-
layer prepreg105
Figure 5.26. Objective funcion change during each iteration of Nelder-Mead algorithm
for 1 layer prepreg106
Figure 5.27. The comparison of the recommended temperature profile and optimized
temperature profile achieved by the Nelder-Mead algorithm for 1 layer prepreg107
Figure 5.28. Tempreature profile parameters evolotion in Nelder-Mead algorithm for 2
layer prepreg108
Figure 5.29. Objective funcion change during each iteration of Nelder-Mead algorithm
for 2 layer prepreg109
Figure 5.30. The comparison of the recommended temperature profile and optimized
temperature profile achieved by the Nelder-Mead algorithm for 2 layer prepreg109

LIST OF SYMBOLS

ū	Darcy's Velocity
μ	Viscosity
К	Permeability
Р	Pressure
ρ	Density
'n	The rate of total mass in control volume
\dot{m}_{in}	The rate of inflow mass
\dot{m}_{out}	The rate of outflow mass
\dot{m}_{sink}	The loss of fluid mass in sink
М	Mass
S	The sink term
Т	Temperature
C_p	Specific heat capacity
k	Thermal conductivity
q_t	Total reaction heat
α	The degree of cure
Ø	Porosity
Øo	Initial porosity
υ	Fiber volume fraction
v_0	Initial fiber volume fraction
\forall_{total}	Initial volume of prepreg
\forall_{fiber}	Initial fiber volume
h_0	Initial prepreg thickness
p	Pressure in a point of domain
p_{0}	Initial pressure in a point of domain
ε	Linear volumetric strain
K ₀	Initial permeability
A _i	Exponential coefficient
E _A	Activation energy
R	Universal gas constant
D	Diffusion constant

α_{C0}	Curing degree at absolute zero temperature
α_{CT}	The increase in critical degree of cure with temperature
m_1, m_2, n_1, n_2	Numerical constant of cure kinetics equation
A, B, C	Numerical constant of viscosity equation
E_{μ_1}, E_{μ_2}	Resin activation energies in viscosity equation
α_{gel}	Degree of cure in gelation point
$arepsilon_p$	Instantaneous porosity of domain in Comsol Multiphysics®
Q_m	Source term in Comsol Multiphysics®
φ	Level Set function parameter
γ	Reinitialisation parameter
\mathcal{E}_{ls}	Parameter controlling interface thickness
$(\cdot)_{eff}$	The indicator for effective form of properties
(·) _{air}	Air property
$(\cdot)_{resin}$	Resin property

Chapter 1

INTRODUCTION

1.1. Out of Autoclave Processes

The underlying reason for usage of composite parts in various industries is to have need for lightweight, high structural strength from the manufactured parts. Example of industries that requested these types of parts, can be given as aerospace, automobile, marine, sport goods etc. [1]. The advancement of composite manufacturing process makes the manufactured parts to be more expensive, and relatively inaccessible for industries that does not have critical need for lightweight and high strength parts such as industries of sport goods, and marine. The repeatable and inexpensive composite manufacturing process for automobile industry is also limits the extensity of composite manufacturing for this industry. However, the importance of composite manufacturing process for aerospace industry is essential to obtain sustainable and effective composite manufacturing process. To overcome the composite manufacturing challenges for the aerospace industry demands, the autoclave process has been introduced and developed over the years to meet the demand by aerospace industry. Basically, the autoclave process is aimed to apply higher temperature and pressure on the manufactured parts with autoclave ovens, which must be as big as the parts being manufactured (Figure 1.1). The geometrical limitations of the autoclave ovens, the requirements of the uniform temperature, pressure distribution over the part, are challenges in the autoclave process that causes increasing in operational costs.



Figure 1.1. Autoclave ovens used for the composite manufacturing [2],[3].

Autoclave composite manufacturing process is appeared to be chosen as a primary composite manufacturing process for aerospace industry. Alternatively, Out of Autoclave (OoA) process started to develop as opposed to autoclave composite manufacturing process. OoA process is a composite manufacturing technique that has been performed with specially manufactured OoA pre-impregnated (prepregs) laminates. The process itself differs substantially in terms of process conditions. The composite parts manufactured with OoA process does not require high temperature and pressure occurrence during manufacturing cycle. The absence of autoclave oven is, maybe, the most significant feature of OoA composite manufacturing process. The geometrical restrictions and operational cost of Autoclave composite manufacturing are also other disadvantages of this process, which limits the number of manufactured parts per time. Besides advantages of OoA, the occurrence of lesser pressure difference and decreased temperature peak in typical OoA prepregs are nonignorable disadvantages of OoA process. Research for OoA composite manufacturing technique, is indispensable field for composite manufacturing community to achieve parts that are compatible to Autoclave manufacturing process. The composite manufacturing techniques for aerospace industry can be divided into two groups, i) Autoclave, ii) Out of Autoclave. These groups for composite manufacturing techniques includes several different composite manufacturing processes. Vacuum Bag Only (VBO) process that will be discussed during this thesis, is one of the OoA manufacturing technique that has potential to be used in order to meet higher manufactured parts demanded by aerospace industry [4].



Figure 1.2. The schematic representation of Aerospace composite manufacturing techniques and the place of Vacuum Bag Only process [4]

OoA processed composite parts are manufactured with pre-impregnated fiber sheets, also known as prepreg. The usage of prepregs in advance composite manufacturing processes is to decrease total impregnation time of fibers, also control over the ratio of resin and fiber in each layer of composite parts. Moreover, manufacturing of composites with molds are also possible with OoA process. Preformed geometries can be used to manufactured various shaped composite parts as well.

In the light of these developments, OoA composite manufacturing processes are an incontrovertible research field. OoA process offers primary advantages compared to the many other composite manufacturing techniques. Researches in order to develop other composite manufacturing processes can be used for VBO process as well and is necessary for future of composite manufacturing. Filling time determination, fiber permeability calculations, pressure distribution and its effects, fiber resin wetting studies, constitute a base for resin flow. Optimum temperature profile for curing, and methodologies of mathematical equation construction for cure kinetics, can also be counted as researches of composite manufacturing processes. Cured part thickness and air removal calculations under low pressure difference conditions, are among valid and important studies. It is vital that developments for VBO process can give great opportunity for many industries.

1.2. Vacuum Bag Only Process

Out of Autoclave manufacturing techniques are the potential manufacturing techniques that have enormous potential to obtain higher manufacturing volumes, to fulfill scalable, controllable and repeatable composite manufacturing processes for the aerospace industry. Among OoA manufacturing techniques, Vacuum Bag Only (VBO) process is the newly developing process, actually started to develop in last two decades [5], that has significant advantages over other techniques. To understand VBO process, VBO manufacturing needs to be introduced from both material handling strategies (layup), and the processing of prepregs.

VBO manufacturing process can be performed with low temperature OoA prepregs [6] without need for autoclave oven. The process can be fulfilled with the oven under atmospheric pressure that has relatively less vacuum pressure compared to autoclave processes. Classical VBO process performed with low temperature OoA prepregs can be seen in Figure 1.4 with layup schematics. To create VBO process conditions, some of the practical manufacturing application should be executed. These applications with meaningful reasons can be explained such as. The vacuum bag that are closed with tacky tapes, provides pressure difference maximum of 1 atm with help of vacuum port. Below vacuum bag, breather fabric ensures the uniform pressure distribution on prepregs. Perforated film is used to regulate air evacuation in prepregs as same function as breathable edge dams that also inhibits resin bleed out.



Figure 1.3. Prepreg processing in Vacuum Bag Only process

VBO prepreg mold placement procedure with layup tooling is presented in Figure 1.3. To further VBO process, the process steps should be investigated, and tried to understand purposes of each steps, so that VBO manufacturing process modelling is correctly achieved. First step of VBO process is started with layup preparation of prepregs that have resin film from top and bottom by peeling off one of films to lay up into mold. In order to put prepregs into mold, the application of cleaner, releaser chemicals to mold have crucial role for both surface quality of cured parts, and reusability of mold. However, releaser films can be used for the same purposes as well. The perforated films that have micro level pores, let air to be evacuated inside prepregs with vacuum pressure. In order to prevent resin bleed out, the edge dams are placed as close as possible so that the resin cannot escape through mold. These edge dams should be breathable so that air can be removed with uniformly distributed vacuum pressure by breather fabric. Finally, the vacuum bag is placed into mold to create close environment to cure prepregs with temperature profile. The steps of VBO manufacturing process is given in Figure 1.4.



Figure 1.4. VBO process steps with Out of Autoclave prepregs

1.3. State of the Art on Vacuum Bag Only Process Modelling

VBO process presents significant advantages compared to any other advanced composite manufacturing processes, such as, reduction in operational costs, unrestricted dimensions of part geometry, relatively fast manufacturing cycle resulted with almost void free parts. Mass production of parts with VBO process is also possible. A successful VBO composite manufacturing process provides limitless part geometry with better mechanical performance (higher fiber volume fraction) while reducing of operational and tool costs. However, this process leads by instantaneous change of several physics that causes to be dominated by in a large number of process variables. The relations of processing variables must be considered to achieve successful VBO composite manufacturing.

The integration of individual physics, such as resin flow, heat transfer and consolidation physics, is an essential composite process modeling consideration. As an example of integrations in composite process modelling, resin flow progressing governed by permeability of fiber architecture, viscosity of resin and pressure difference, also changes fiber volume fraction instantaneously that leads thickness change in fiber beds. During curing cycle, the resin system releases heat as exothermic reaction due to chemical characteristics of its. Dissipation of heat over prepregs causes sudden changes in viscosity of resin that also changes resin flow in porous media. The temperature design for both curing and resin flow, and relation of resin flow with consolidation, are some of the composite process modelling problems in order to increase effectiveness of composite manufacturing processes.

Repeatability and sustainability of composite manufacturing is desired for most of composite manufacturers, especially, critical parts manufacturers. Engineered processes for specific prepreg systems with optimized manufacturing cycle, attains manufacturers to get void free parts, better mechanical performance, at least parts that are in limitations for various standards. The systematic studies for composite manufacturing process contribute to construct scalable, controllable and repeatable processes. Computational methodologies for composite manufacturing processes can be used for improving process outcome and helped to optimize overall processes. In literature, resin flow, curing time and cured thickness determinations are already available for various composite manufacturing process. These methodologies involve complex engineering equations,

and hard to handle. By using math and physics, composite manufacturing modelling approach can give great benefit to accomplished scalable, repeatable and controllable VBO process solutions with void reduced parts. State of art on VBO manufacturing process will be given below with literature review.

The number of composite parts demanded by industry, is increasing by sectors such as automotive, wind turbine, marine, and aerospace industries [1]. The development of composite manufacturing processes for various industries become important phenomena in order to satisfy industry in the sense of controllable, scalable and repeatable manufacturing processes. In particular, lightweight critical structural components of the aerospace industry are usually manufactured with an autoclave process that requires high pressure and temperature in autoclave ovens, making void free components in return for increasing operation costs with geometrical restrictions. In parallel to these developments, Out of Autoclave (OoA) manufacturing technique with Vacuum Bag Only (VBO) methods [4] ensures elimination of required initial investment for autoclave oven, reducing resin impregnation time and efficient energy consumption with effective cure cycles, that results promising void reduced parts [5]. However, the vacuum pressure applied in OoA process is a maximum of 1 atm, and process parameter determination for specific prepreg types, is extremely important in order to reach Autoclave quality with OoA prepreg systems. Ineffective completion of OoA process causes obvious reduction of mechanical performance of final cured parts as mentioned in literature [7].

The engineered vacuum channels (EVaCs) is one of the prepreg design strategies to eliminate voids by letting air evacuated from dry region of prepreg [8]. Other than EvaCs, the right process conditions for OoA prepregs depending on resin and fiber types are essential manufacturing consideration. Effective process parameter determination techniques are among the challenges in the composite manufacturing community due to the complexity of physics in OoA process. Furthermore, the complete OoA process is simultaneously governed by a combination of flow, heat and consolidation physics in addition of time dependent parameters of fiber architecture and resin systems. The complexity of OoA manufacturing technique with VBO method is unable to predict quality of OoA process for specific prepreg systems. Therefore, the quality assessment parameter in literature has been focused on void content [9], [10], [11], [12].

The present studies in the literature have been introduced with significant contributions in order to explain VBO process of governing physics and parameters. The numerical approaches used to evaluate VBO process varies different aspects of the actual process such as resin flow, heat transfer, and consolidation, either individual or coupling of these individual (multiphysics) physics. Resin flow based studies, mostly focused to exhibit void formation of prepregs that is resulted with mass (pores, air, moisture) and momentum (intra tow pores) transfer during flow [13]. Reduced porosity with different environmental conditions such as moisture [9], out time effect [8], fiber architecture [14] is contributed to developed mathematical modelling of resin flow in prepregs. Effective parameters that control resin flow, such as permeability [15], viscosity [6] and pressure drop [16], have been performed. Thomas et. al. obtain through thickness permeability of vacuum bagged prepregs by using ultrasonic imaging C-scan to utilize a density map in prepreg [15]. Grunenfelder et.al. investigated the effect of moisture [9] and out time effect at room temperature [8] on void formation inside prepregs and found that these parameters in the manufacturing are a significant factor for void formation inside prepreg in OoA. Centea et al. evaluated impregnation of resin during different levels of curing of OoA process with Micro-CT, concluded as the curing time increased, voids in the prepreg decreased [11], also studied material properties and process parameters on tow impregnation of three different prepreg system [12]. Xin et al. proposed in plane and through thickness air permeability measuring methodology, concluded that temperature and compacting pressure are crucial parameters for void defects for OoA prepregs [10]. Kourkoutsaki investigated modeling of impregnation by coupling resin and air flow separately, concluded delayed air evacuation case successfully validates impregnation time of tow [13].

Another main physical result of VBO manufacturing is the consolidation of prepregs during resin infiltration. Total thickness of prepreg is decreased due to fiber bed compaction with progression of the resin flow front inside prepreg. The relation of air flow with resin flow is attracted attention in order to clarify air escaping mechanism with transport approaches [13],[17],[16],[18]. The consideration of air flow coupled with resin flow appeared to be an essential parameter that causes to increase porosity in final cured parts. Helmus et.al. evaluated consolidation coupled with air evacuation and impregnation. Total thickness change of prepreg with air evacuation and curing formulations is described as a function of fiber volume fraction and compaction pressure that validated experimentally [19]. This studied is extended with a stochastic flow front position study to forecast impregnation related final consolidation of prepregs as well [20]. Gangloff et al. developed a mathematical model to obtain the prepreg's final thickness for compaction of OoA partially impregnated prepregs by considering less and more air pathways [21]. Continuum approach for consolidation as used in other composite manufacturing processes, is applied for VBO [22] that considers volatile dissolving and its transports with Henry's Law coupled with Terzaghi's equations.

Besides resin flow and consolidation physics, cure kinetics and thermal properties of OoA process are investigated in the literature. OoA prepreg systems are designed to start curing relatively in low temperature ranges (80-130°C) [23] that is followed by higher post cured ranges up to 180°C. Special chemical composition of OoA resin systems shows different cure kinetics characteristics compared to other composite manufacturing resin systems. Kratz et al. developed a cure kinetics model for commercially available OoA prepreg systems based on DSC results to predict thermal characteristics [6]. Kim et al. investigated aging effects of neat resin and prepreg to obtain cure kinetics and viscosity change [24], and use dielectric cure monitoring method to predict the instant degree of cure, cure rate, and viscosity [25]. Dong et al. proposed an optimized cure cycle determination methodology based on cure kinetics, viscosity, DMA and TGA results, found that sample manufactured with optimized cycle gives better mechanical performance [26]. Hwang et. al. obtain an optimized temperature profile by using cure kinetics, viscosity models in order to accomplish higher fiber volume fraction [27].

Nevertheless, extensive researches in the literature show great harmony numerically as well as experimentally. A fully integrated numerical methodology for the VBO process has not been achieved in literature, even though, the coupling of resin flow and consolidation physics are available. The multiphysical modeling of VBO composite manufacturing with integration of resin flow, heat transfer and consolidation can help to improve repeatable, controllable and scalable process for void restricted industries. This study aims to develop an multi physical modelling for VBO process coupled with resin flow, heat transfer and consolidation physics to achieve cured parts with lesser void content. Achieved multi physical model is used for numerical tests of 1, 2, and 4 layers of prepreg, then temperature profile parameters are subjected to parametric study. The change of void content with ranges of different parameters is obtained. Additionally, the

void initiation mechanism during VBO process is attained that shows the development of air evacuation channels evolving to bubbles during impregnation.

1.4. Scope and Organization of the Thesis Study

In this thesis, OoA composite manufacturing technique for VBO method is investigated in order to identify effective processing parameters. Parameters of governing physics and emprical relations used to interpret OoA process is integrated to construct mathematical model in order to utilize optimized manufacturing cycle of OoA process. Integrated OoA process modelling coupled with resin flow, heat transfer and consolidation physics are developed in order to minimize void content of final cured parts, hence, maximization of mechanical performance. The developed model is used to identify right process conditions such as temperature profile parameters (dwell time, upper and lower temperature limits, ramp rate, etc). Developed model that solved with commercial software, is subjected to parametric and optimization studies.



Figure 1.5 The followed systematic for the development of multiphysical VBO process modeling

The developed model includes three different governing physics. The resin flow is solved with viscous flow through porous media, Darcy Law. Cure kinetics and volume averaged heat transfer in porous media is solved with modified general heat transfer equation. The consolidation physics is obtained with continuum approaches used in literature [22]. The integration of each parameters of governing physics assures that complete VBO manufacturing process have been achieved.

First chapter of this thesis, the description of OoA composite manufacturing technique have been introduced to identify the purposes of thesis. The relation of OoA manufacturing technique with VBO method is presented. The need for integrated modelling of VBO process is explained with summary of current literature knowledges.

In the second chapter of this thesis, theoretical explanations of governing physics in VBO are presented and, mathematical model development steps are explained with relations of actual physics behind VBO process. Equation parameters in multiphysical perspective is given.

In Chapter 3, obtained mathematical models is implemented via commercially available software COMSOL Multiphysics[®]. The implementation of physics stated in Chapter 2, is given for both individually and integrated way. Boundary conditions that mimics VBO process, are also presented.

In Chapter 4, the optimization study with COMSOL Multiphysics® is implemented with Nelder-Mead algorithm. The objective function definition, the constraints definition with selection of VBO process parameters is discussed. In order to understand the algorithm working principle, the case study, i) the new created problem, ii) implementation on 1-layer VBO prepregs, are performed in this chapter.

In Chapter 5, the result of developed and implemented model is given and discussed in this section. Integration of resin flow, heat transfer and consolidation physics are shown. However, the developed model is extended to be used for optimization study as well as 1-layer, 2-layer and 4-layer of prepreg systems. The multiphysical assessments of developed model and the parametric solution for VBO process parameters, and the optimization results are revealed and discussed.

In Chapter 6, the results of parametric studies, and optimization studies are summarized, and significant findings of results are discussed. The parameter determination strategy for OoA prepregs are shown according to the multiphysical VBO process model integrated with resin flow, heat transfer and consolidation that is developed in this thesis. Future work in contribution to develop VBO process is also given in this chapter.



Figure 1.6.Pert chart of the thesis study

Chapter 2

MODELING OF VACUUM BAG ONLY PROCESS

In this chapter of this thesis, defined composite manufacturing process, VBO, is explained first physically and then mathematically. Detail description of mathematical models for the resin flow, the heat transfer and the consolidation physics, is given. Governing equations and empirical relations are expressed to link physics and mathematics for VBO process.

2.1. Vacuum Bag Only Process Modelling

The nature of VBO process requires the integration of various physics. These physics mathematically are represented with the governing equations that involves a lot of different parameters. The parameter map for the flow, heat transfer and consolidation physics are shown in Figure 2.1. The multiphysical approach is needed to consider due to the number of parameters required to calculate the instantaneous void content of prepreg. The relationship between these physics, the integration for the common parameters, has to be clearly determined before the calculation. The change of material properties that caused by one physics, also can affect other physics as well. The material property for each time increment might be updated. Therefore, the parameters specific to individual physics, the common parameters used by several physics and the coupling of the governing physics will be explained one by one in this section of the Chapter 2.

The resin and the fiber architecture are the main elements of the prepregs. The resin is initially viscous fluid that should be in a condition where the fluid can diffuse into fibers during processing. On the other hand, in composite manufacturing processes, the vacuum pressure application is often used to supply the movement of the resin. In micro level, the position and the distance of the fibers with respect to each other is also effective parameter for the flow of the resin, which is related with the fiber structure of the prepreg. Basically, the flow of the resin system along with fiber architecture is one of the main physics that has to be solved for multiphysical VBO manufacturing process. The flow in shows Darcy's Law parameters that requires to handle the viscosity, the permeability, the pressure difference, and the porosity to find the velocity of the resin through porous media and the instant porosity.

The temperature profile application in VBO process benefits on several physical advantages. Knowing the resin viscosity and the degree of cure in any time of manufacturing cycle can only be acquired with the control of Heat Transfer equation. The effect of temperature profile over the prepreg is also governed with this equation (Figure 2.1.). The properties to calculate temperature distribution over the prepreg can be predicted by knowing the conductivity, the specific heat capacity and the density for the resin and the fiber that are to be used volume averaged in solution domain. Besides temperature distribution, the viscosity and the cure kinetics equations are calculated with the coupling of Heat Transfer equation. The initial, degree of cure, and empirical equation parameters are needed to be defined.

The consolidation due to vacuum hold under bag constitutes the thickness change of the prepreg during VBO processing. However, the vacuum bag pressure is not just effective physics in consolidation. While the resin flows through the fibers, the air flow also initiated. The air evacuation due to the resin flow also fulfills the consolidation in prepreg. The gas volume under temperature and pressure described by Henry's Law that one can use to interpret the volume of air, thereby, the porosity in prepreg. This equation will be used to find the volumetric strain due to temperature, pressure (Figure 2.1.). However, the velocity of the resin that ensures the impregnation during VBO manufacturing process conditions. The aim of the consolidation calculation yields to find the final prepreg thickness.

The material properties such as porosity, temperature of the prepreg, are dynamic parameters during VBO process. The initial porosity value is used in the flow calculation as well as in consolidation. Heat transfer equation finds temperature distribution over prepreg and the viscosity is also function of temperature and the degree of cure. The flow equation should be coupled with the heat transfer equation. The properties that are calculated with the individual physics, can be used in another physics simultaneously, so the physics should be integrated with each other. The multiphysical integration for the VBO manufacturing process is achieved with the map shown in Figure 2.1. Detail equation forms for all calculations will be explained in further sections.



Figure 2.1.The defined and solved parameters in multiphysical modelling of VBO process

2.2. Flow through Porous Media

The flow of resin in composite processing is defined as viscous flow through porous media. In literature [1], Darcy Law used to describe resin flow inside fibers. Basically, volume averaged resin viscosity is correlated with averaged fiber permeability under pressure difference. Derivation of Darcy Law comes from derivation of conservation of momentum equations with assumptions of volume averaged viscous stress of flow [28]. The simplified equation of conserved momentum equation of viscous flow reduced into:

$$\bar{\mathbf{u}} = -\frac{\mathbf{K}}{\mu} \cdot \nabla \mathbf{P} \tag{2.1}$$

Where \bar{u} is local viscous flow velocity under pressure gradient (∇P), μ viscosity of resin, K permeability of fiber networks. This equation is acceptable for each axis of flow in macroscopic level. Darcy Law simplifies overall momentum equation calculations for each channels of fiber networks by providing relationship between pressure drop and averaged velocity.



Figure 2.2. Schematic of permeability concept

The directionality of flow is basically determined by permeability (K) of fiber architecture. The permeability term in Darcy Law is a tensor rather than scalar value. Figure 2.2 shows that the permeability effects on resin flow for 2D. Controlled fiber volume is subjected to injected resin, where injection occurs in 3 principle axes. The three cases show comparison of dominated axes permeability values. The 3D vectoral form of Darcy Law can be seen in Equation [2.2].

$$\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = -\frac{1}{\mu} \begin{pmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{pmatrix} \begin{pmatrix} \partial P / \partial x \\ \partial P / \partial y \\ \partial P / \partial z \end{pmatrix}$$
 [2.2]

The conservation of initial resin quantity is essential mathematical equations for porous flow in order to calculate instantaneous resin velocity or resin flow front. The conservation of mass, also known as continuity equation, in composite manufacturing processes, especially for VBO process, is presented based on transport equations that will be shown by using a unit volume element approach during impregnation of resin.

If we consider a fluid flow in defined volume $(\Delta x \Delta y \Delta z)$ with a density (ρ) and velocity (U). In the cartesian coordinate system, velocity and density of fluid can be defined as function of x, y, z and time, so represented as U(x, y, z, t) and $\rho(x, y, z, t)$, also if there is sink which causes to loss fluid mass s(x, y, z, t). The mass of fluid in this control volume, \mathcal{V} at any time, is calculated by integrating density $\rho(x, y, z, t)$ within upper and lower band of \mathcal{V} . From this basic definition of density and velocity, the conservation of mass, or continuity equation can be derived. Here, the balance of mass increase inside control volume $(\mathcal{V}, \Delta x \Delta y \Delta z)$, is derived step by step.



Figure 2.3. Representative control volume of fluid for conservation equations during impregnation of resin

The mass conservation of a fluid in defined control volume can be written in terms of inflow, outflow fluxes, and additionally assumed to have sink term. The change of fluid volume inside predefined volume ($\Delta x \Delta y \Delta z$) is calculated by subtracting change of outflow and mass lost due to sink from change of inflow flux.

$$\binom{Rate \ of}{mass \ increase} = \binom{Rate \ of \ mass}{inflow \ flux} - \binom{Rate \ of \ mass}{outflow \ flux}$$

$$= \binom{Rate \ of \ mass}{lost \ from \ sink}$$

$$[2.3]$$

$$\dot{m} = \dot{m}_{in} - \dot{m}_{out} + \dot{m}_{sink} \tag{2.4}$$

The surface of control volume (x, y, z) is fixed, which means control volume axis, does not change with time. The rate of total mass in control volume (\dot{m}) can be expressed in Equation [2.5]. Since, the density of fluid is known, one can calculate, for example, rate of inflow mass as $(\rho u_x|_x)\Delta y\Delta z$ for x axis, also incremental change of volume in same axis can be expressed $(\rho u_x|_{x+\Delta x})\Delta y\Delta z$. The subtraction of inflow and outflow mass change for each axis is stated in Equation [2.6].

$$\dot{m} = \frac{\partial M}{\partial x} = \frac{\partial}{\partial t} (\rho \Delta x \Delta y \Delta z) = \frac{\partial \rho}{\partial t} \Delta x \Delta y \Delta z$$
[2.5]

$$\dot{m}_{in} - \dot{m}_{out} = \Delta y \Delta z (\rho u_x|_x - \rho u_x|_{x+\Delta x}) + \Delta x \Delta z (\rho u_y|_y - \rho u_y|_{y+\Delta y}) + \Delta y \Delta x (\rho u_z|_z - \rho u_z|_{z+\Delta z})$$
[2.6]

The loss of fluid mass at rate of s(x, y, z, t) per unit time within \mathcal{V} is given in Equation [2.7]. *s* is volume averaged loss of mass.

$$\dot{m}_{sink} = \int s(x, y, z, t) d\mathcal{V} = s \Delta x \Delta y \Delta z$$
[2.7]

After achieving each parameter of Equation [2.3], the substitution of Equation [2.5], [2.6] and [2.7] gives Equation [2.8].

$$\frac{\partial \rho}{\partial t} \Delta x \Delta y \Delta z = \Delta y \Delta z (\rho u_x |_x - \rho u_x |_{x + \Delta x}) + \Delta x \Delta z (\rho u_y |_y - \rho u_y |_{y + \Delta y}) + \Delta y \Delta x (\rho u_z |_z - \rho u_z |_{z + \Delta z}) - s \Delta x \Delta y \Delta z$$
[2.8]

In order to rearrange Equation [2.8], dividing both side of equation by control volume, $\Delta x \Delta y \Delta z$ yields to Equation [2.9]. While $\Delta x, \Delta y$ and $\Delta z \rightarrow 0$, convergence of Equation [2.9] gives Equation [2.10].

$$\frac{\partial \rho}{\partial t} = \frac{(\rho u_x|_x - \rho u_x|_{x+\Delta x})}{\Delta x} + \frac{(\rho u_y|_y - \rho u_y|_{y+\Delta y})}{\Delta y} + \frac{(\rho u_z|_z - \rho u_z|_{z+\Delta z})}{\Delta z} - s \quad [2.9]$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(\rho u_x) - \frac{\partial}{\partial y}(\rho u_y) - \frac{\partial}{\partial z}(\rho u_z) - s \qquad [2.10]$$

$$\frac{\partial \rho}{\partial t} + \nabla . \left(\rho U\right) + s = 0$$
[2.11]
The partial derivation of density $\frac{\partial \rho}{\partial t}$ at fixed volume can be written in the form of continuity equation as substantial derivative $(D\rho/Dt)$. Open form of substantial derivative of continuity equation for fluid flow is shown in Equation [2.12].

$$\frac{D(\cdot)}{Dt} = \frac{\partial(\cdot)}{\partial t} + \frac{\partial(\cdot)}{\partial x}\frac{dx}{dt} + \frac{\partial(\cdot)}{\partial y}\frac{dy}{dt} + \frac{\partial(\cdot)}{\partial z}\frac{dz}{dt}$$

$$= \frac{\partial(\cdot)}{\partial t} + \frac{\partial(\cdot)}{\partial x}u_x + \frac{\partial(\cdot)}{\partial y}u_y + \frac{\partial(\cdot)}{\partial z}u_z$$

$$= \frac{\partial(\cdot)}{\partial t} + U.\nabla(\cdot)$$
[2.12]

The substitution of Equation [2.11] into Equation [2.12] and rewrite expression of $\nabla \rho U = \nabla \rho U + \rho \nabla U$, then obtained Equation [2.13]. Fluids in composite manufacturing processes generally assumed to be constant during processing time as quasi-steady state, so the density change $(\frac{\partial \rho}{\partial t} = 0)$. However, most of the time the sink effect will not significant during process (s = 0). The conservation of mass during composite manufacturing can be simplified as in Equation [2.14].

$$\frac{D\rho}{Dt} + \rho \nabla . U + s = 0$$
[2.13]

$$\nabla . \, U = 0 \tag{2.14}$$

2.3. Heat Transfer in Out of Autoclave Prepregs

One of the main physics in composite manufacturing processes is heat implementation during processing of matrix. The applied temperature profile has vital effect on several properties of prepreg such as degree of cure, viscosity, glass transition temperature etc. Especially, the effect of mechanical performance and void initiation mechanism in resin rich regions of prepregs with various temperature profile application studies have been examined under title of heat transfer in composite manufacturing processes. Also, the effect of temperature profile on void volume, shape and distribution is known by literature studies [29]. For example, the viscosity of resin leads to establish air evacuation channel during resin flow due to applied cure cycle or temperature profile. The non-optimized cure cycles can yield this evacuation channels to be closed before fibrous medium fully filled with resin, that appears undesired void content in final cured parts.

In order to construct the Heat transfer mathematic, several material properties for fiber architecture and resin system must be known such as densities, specific heat capacities, thermal conductivity etc. These parameters are important for temperature distribution over the prepreg and effect of applied temperature on the manufactured parts. In order to understand, and observe, cure kinetics and viscosity of specific resin system under various temperature profiles. In the scope of this thesis, temperature profile application will be investigated with general heat transfer equation in addition to source term that exothermic reaction heat appears due to increase in degree of cure, often used [27],[23],[30].

$$\rho C_p \left(\frac{\partial T}{\partial t} + \bar{\mathbf{u}} \cdot \nabla \mathbf{T} \right) = \mathbf{k} \nabla^2 \mathbf{T} + q_t \frac{d\alpha}{dt}$$
[2.15]

Where ρ prepreg volume averaged density, C_p specific heat capacity, T temperature, t time, \bar{u} Darcy's velocity, k thermal conductivity, q_t total reaction heat and $d\alpha/dt$ cure rate. General Heat transfer equation will be basis to observe temperature profile effect on cure kinetics and viscosity of resin system.

2.4. Consolidation in Vacuum Bag Only process

The consolidation in VBO process is issued by several parameters, for example, fiber bed compaction, air evacuation ratio and resin impregnation degree etc. [19] (Figure 2.4). During VBO process, OoA prepregs are placed on the top of each other, and then vacuum pressure applied with the maximum of 1 atm under vacuum bag. The initial thickness of prepreg reduces as soon as the vacuum pressure applied. The reaction of fiber bed due to this vacuum pressure called fiber bed compaction. In curing cycle, the resin viscosity starts to reduce so that the impregnation of resin through prepreg in consequences of temperature profile resulted with increasing of the impregnation degree of prepreg. The

increasing in fiber volume fraction and the decreasing of porosity causes to thickness reduction in prepreg. The resin flow that is initiated with pressure drop and change of viscosity, Darcy Law parameters, creates the air flow that propagates air evacuation in dry spots of prepreg. The visuals of initial, impregnation and final stages of prepreg during VBO manufacturing are presented in Figure 2.5.



Figure 2.4. The leading mechanism of VBO prepreg consolidation

Ready to use prepregs doubtlessly have porous that causes in various reasons, for example, lack of compaction pressure where resin film and fiber sheets meet in the roller of prepreg manufacturing lines, resin film itself may have entrapped air bubbles too [21]. Hence, porosity in prepreg during manufacturing and after manufacturing, will be inside cured parts. The main consideration in composite manufacturing process, particularly, VBO process, is to prevent voids that can caused due to processing conditions.

During impregnation, the resin flow front simultaneously progresses due to applied temperature profile that reduces viscosity of resin and fills empty spaces of fiber sheets. Since, the initial fiber volume fraction and porosity are dependent variables with each other (Equation [2.16]). However, the fiber volume fraction experimentally calculated based on the ratio of fiber content to resin and air inside the prepreg, so if resin is impregnated along the porous domain of prepreg, the fiber volume fraction and porosity will change with the time (Figure 2.5).



Figure 2.5. Representation of air pore change during consolidation while impregnation

Due to vacuum bag compaction pressure, prepreg layers subjected to pressure that causes reduction of prepreg thickness during process. Eventhough, the thickness change, also known as consolidation occurs, the total fiber content will not change in prepreg. Initial fiber volume content (v_0) theoretically is the ratio of initial volume of prepreg \forall_{total} to initial total fiber content \forall_{fiber} . The total volume of prepreg can be calculated by multiplying the area of initial resin impregnated area with initial thickness of prepreg layer($\forall_{total} = A. h_0$). Therefore, the fiber volume fraction as a function of prepreg layer thickness can be calculated with Equation [2.16].

$$v(t) + \phi(t) = 1$$
 [2.16]

$$1 - \emptyset(t) = v(t) = \frac{\forall_{fiber}}{A.h(t)}$$
[2.17]

These formulations are not just enough to describe realistic consolidation behavior of VBO manufacturing process. Literature studies show that the temperature profile parameters such as ramp rate, dwell time are effective parameters for consolidation [19], [14]. These parameters define resin impregnation time by determining viscosity so that the fiber volume content and porosity of prepreg varies accordingly. The continuum approach to obtain instant thickness change related with total volume change have been defined in literature [22], [31].

$$\frac{\phi p}{T} = \frac{\phi_0 p_0}{T_0}$$
[2.18]

$$\phi_0 + \varepsilon = \phi \tag{2.19}$$

$$\varepsilon = \frac{\phi_0 p_0 T}{p T_0} - \phi_0 \tag{2.20}$$

In order to relate porosity and temperature profile, the porous or volatiles, which are filled with air, assumed to follow ideal gas law during process. The porous in prepreg are not dissolvable and be formed of bubbles. The volume, temperature and applied pressure can be described with Henry's Law for any location of prepreg (Equation [2.18]). Relation of porosity with deformation can be calculated by substituting Equation [2.19] into Equation [2.20], where initial temperature, pressure, porosity (T_0 , p_0 , ϕ_0), instantaneous (T, p, ϕ), linear volumetric strain (ε) is expressed.

Due to compaction pressure applied by vacuum bag, the total thickness of prepreg decreases with time, which also meant to be decreasing in total volume of porous media. As a result of volume change, the length between each fiber pieces in micro level, have shorten that causes to reduction in impregnation time of porous domain. Moreover, calculation of fiber volume fraction depends on the volume of individual resin and fiber amounts. In any change of initial volume of prepreg yields to change in fiber volume fraction in macro level.

The permeability calculation with respect to fiber volume change, as often used in literature [32],[33], [34], have been implemented to get instantaneous permeability of porous media. In above approaches in micro and macro level, the permeability of VBO prepregs is calculated with Kozeny-Karman relation. The initial permeability (K_0) of porous domain, and time dependent fiber volume fraction (v(t)) is enough to calculate permeability with Kozeny-Karman equation (Equation [2.21]).

$$K(t) = K_0 \frac{(1 - v(t))^3}{v(t)^2}$$
[2.21]

2.5. Equations of Empirical Relations

The empirical relations are used in developed model in order to model VBO manufacturing process with multiphysical approach. The material behavior for specific properties are expressed with the empirical relations. Indeed, the physical properties are stated mathematically by using these empirical relations. In the scope of thesis, the empirical relations are used for the cure kinetics and the viscosity models, respectively.

Understanding of thermo-chemical feature of resin system have a vital effect on the success of inter and intra tow resin flow, optimizing total process time and implementation of uniform temperature distribution resulted with uniform curing over the part, etc. The designed temperature profile should be considered for a resin system which determined based on its own characteristic. The chemical composition of resin system varies one another due to different amounts of chemical hardeners included polymer molecules. Therefore, the good interpretation of cure kinetics characteristic of resin relies on successful mathematical models, which covers realistic experimental tests performed under dynamic and isothermal conditions. After achieving mathematical model, one can get cure kinetics and degree of cure of the resin system without the need for experiments steps because of these developed mathematical cure kinetics models.

The modelling of cure kinetics equation in this thesis is used in the form of Equation [2.22]. The equation developed for low temperature OoA prepregs, which implemented degree of cure, glass temperature, and viscosity and validated on the example of thick section parts [6]. Experimental curing rate and parameters used to fit diffusion controlled an autocatalytic equation developed by Cole et al. [35]. The equation expressing cure kinetics of resin system is given below:

$$\frac{d\alpha}{dt} = K_1 \alpha^{m_1} (1 - \alpha)^{n_1} + \frac{K_2 \alpha^{m_2} (1 - \alpha)^{n_2}}{1 + e^{\left(D(\alpha - (\alpha_{C0} + \alpha_{CT}T))\right)}}$$
[2.22]

$$K_i = A_i e^{\frac{-E_{A_i}}{RT}}, \quad i = 1,2$$
 [2.23]

Where A_i exponential coefficient, E_A activation energy, R universal gas constant, T absolute temperature, D diffusion constant, α_{C0} curing degree at absolute zero temperature, α_{CT} the increase in critical degree of cure with temperature, and m_1 , m_2 , n_1 , n_2 are numerical parameters.

The heat transfer application as oven curing in VBO process provides successful impregnation of resin through porous domain with temperature profile that is specifically designed for resin system. Lowering resin viscosity with initial curing temperature parameter ensures impregnation of resin along with porous media. However, degree of cure, and gelation are important parameters for viscosity. While resin starts to reduce its viscosity, as a result of temperature increase in prepreg, degree of cure is increased in addition to exothermic reaction that yield increasing in viscosity as well. The gelation point of resin system also, determines a point where resin viscosity is no longer concern of impregnation, because the prepreg system started to cure which is irreversible.

Mathematical modelling of resin viscosity is dependent with the temperature, degree of cure, gelation point. In this study, the equation that is developed for fast cure OoA resin systems, have been implemented for the viscosity of resin, which coupled with heat transfer and degree of cure equations (Equation [2.24]). The resin system used in VBO prepreg have been characterized based on set of dynamic and isothermal rheometer test results. Experimental viscosity results is fitted a equation that includes gelling parameters developed by Khoun et al. [30].

$$\mu = A_1 e^{\frac{E_{\mu_1}}{RT}} + A_2 e^{\frac{E_{\mu_2}}{RT}} \left(\frac{\alpha_{gel}}{\alpha_{gel} - \alpha}\right)^{A + B\alpha + C\alpha^2}$$
[2.24]

Where A_1 and A_2 exponential constant, E_{μ_1} and E_{μ_2} resin activation energies, R universal gas constant, *T* absolute temperature, degree of cure α , at gelation point α_{gel} , and A, B, C are fitting constants.

Chapter 3

NUMERICAL IMPLEMENTATION

The numerical solution of multi-physical modelling of VBO process with commercial OoA prepregs is studied by using COMSOL Multiphysics® software that includes built in functions for wide range of physics. It has capability to construct solution for well-known partial differential equations, and also enables user to intervene, or redefine the scientific or engineering problems, which can be easily coupled with this software by the help of user-friendly interface. COMSOL Multiphysics® is especially useful to implement multi-physical engineering problems that nowadays almost all of them requires. The details of COMSOL Multiphysics® software can be found in their reference manuals with industrial applications [36].

The mathematical description of VBO process with governing physics of the process have been presented in Chapter 2. Multi-physical nature of VBO process obligates to handle several physics, that are resin flow with Darcy's Law, temperature profile effect with General Heat Transfer, and consolidation with Arbitrary Lagrangian-Eularian Method (ALE). In addition to these physics, the tracing of instantaneous resin flow front is solved with Level Set equation coupled with Darcy's velocity. The equation for cure kinetics is solved with another COMSOL Multiphysics® module, General PDE. The list of software module used for multi-physical VBO process modelling can be seen in Table 3.1. This chapter will present the implementation of governing physics that is shown in Chapter 2, and also explain modifications of built-in COMSOL Multiphysics® equations.

Physics	COMSOL Multiphysics [®] Modules
Resin flow	Darcy Law
Flow front tracking	Level Set Equation
Temperature profile	General Heat Equation
Cure kinetics	General PDE module
Consolidation	ALE (Arbitrary Lagrangian-Eularian)

Table 3.1. Built in modules in COMSOL Multiphysics ®

3.1. Darcy Law

The Darcy's Law (Equation [2.1]) coupled with continuity equation (Equation [2.14]) for a fluid flow, offers a complete mathematical modelling opportunity, that is used various industrial applications such that the pressure gradient is the main driving force. Since the Darcy's Law runs with the volume averaged fluid flow properties such as velocity, density, pressure and ratio of porous in the domain. The computational domain is expressed with volume averaged properties of fluid (resin) and porous media (fiber) in any point of this domain. The numerical solution of porous media flow can be solved in the Comsol Multiphysics[®] program by Darcy's Law formulation in the Fluid Flow module under Porous Media and Subsurface Flow section. The existence formulation for Darcy law and the mass conservation in this section enables user to define the density, viscosity, porosity and permeability tensor values properties, also allows adding source term (Q_m) that can provide the mass conservation in computation domain.

$$\frac{\partial}{\partial t} \left(\varepsilon_p \rho \right) + \nabla \cdot \left(\rho \left(-\frac{\mathbf{K}}{\mu} \cdot \nabla \mathbf{P} \right) \right) = Q_m \tag{3.1}$$

Where ε_p instantaneous porosity of domain, ρ volume averaged density, K permeability tensor (isotropic or anisotropic), μ viscosity of resin, and Q_m source term. The boundary condition for flow and pressure inlet, outlet, and slip boundary, and symmetric boundaries can also be mathematically defined for each boundary. The software allows to interfere each parameters of Equation [3.1].

3.2. Flow Front Tracing Using Level Set Method

The consolidation solution of the Prepreg system includes an expanding flow area with a free surface. Therefore, it is necessary to track the resin flow front simultaneously for multiphysical VBO process. The Level Set Method (LSM) is a method to define interface between two fluid by assigning the zero-level set of a smooth function of these two fluids, in our application, the resin and air interface that the flow fronts are to be tracked. Although the conservation equations are not considered in this method, the calculation algorithm is relatively easy, and the solution is performed on a fixed mesh [37]. A distance function (Equation [3.2]), called the Level Set function, assigns each point in the computational domain with a value representing the shortest distance to the interface that changes zero to one in between two fluids moving interface [38]. The Level Set function, ϕ , is a scalar parameter calculated with the local flow rate without affecting the flow. During the calculation of the position of the interface, and also the position of fluids in certain regions are calculated depending on the Level Set function parameter (ϕ). The LS method for determining the interface can be performed after the flow equation calculated over computational domain during the progression of fluid. Therefore, the advection of fluid velocity equation that comes from Darcy's Law, can be used to define the motion of the level set function and thus the progression of the interface over time.

In this study, tracking of the porous media flow of the resin system by Comsol Multiphysics[®] 5.4 that was carried out with the Level Set formulation defined in the Moving Interface section under the Mathematics module. The Level Set function is defined for the entire computational domain with smoothed Heaviside function whose value varies between 0 and 1. In resin-wetted areas, this function takes the value 1, while

in empty areas takes the value 0 in the interface zone (Figure 3.1). Level Set parameter (φ) at where the value is 0.5, defined as flow front in computation domain.



Figure 3.1. The representative section of level set parameter (φ) progression between two fluids [39]

$$\frac{\partial \phi}{\partial t} + \boldsymbol{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(\varepsilon_{ls} \nabla \phi - \phi (1 - \phi) \frac{\nabla \phi}{|\nabla \phi|} \right)$$
[3.2]

The left hand side of Equation [3.2] gives the motion of the interface, while the right hand side of it are required for numerical stability of Level Set function [39]. ε_{ls} (m) parameter determines the thickness of the interface region, and should be wirtten with respect to a length of smallest mesh in computation domain, as reccomended [36]. Reinitialisation parameter (γ (m/s)) determines the velocity of defined interface between fluids that has to be selected specific to each problem, otherwise the LSM function can give ossilations in interface, or does not even converges. A suitable γ value can be defined as the value of maximum velocity field in computational domain.

After explaining LSM function with effective parameters, this function should proceed with the velocity profile that is resolved from Darcy's law. This solution involves the replacement of in porous domain with resin, because of the fact that the density (Equation [3.3]) and viscosity (Equation [3.4]) in domain should be defined in terms of Level Set parameter (ϕ).

$$\rho = \rho_a + \phi(\rho_r - \rho_a) \tag{3.3}$$

$$\mu = \mu_a + \phi(\mu_r - \mu_a) \tag{3.4}$$

For the level set function, the velocity profile required for convection of Darcy's velocity in the computation domain is assigned as the velocity profile resolved in Darcy's Law. The Darcy velocity is a superficial velocity, and the determination of flow front in the porous medium is obtained by dividing the Darcy velocity by the porosity which is actual velocity. For this reason, the velocity in the computation domain for Level set function is defined as 'dl.u / dl.epsilon' and 'dl.v / dl.epsilon', which "dl.u" and "dl.v" are the axial components of superficial Darcy's velocity, "dl.epsilon" indicates instant porosity of domain.

3.3. Heat Transfer in Prepregs

Heat Transfer equation for temperature profile effect in prepreg systems can be solved with "Heat Transfer in Porous Media" module under the name of "Heat Transfer "section in Comsol Multiphysics® software. The form of the equation in this module is used to cover the weight distribution of the fiber and resin in the porous medium of the General Heat Transfer equation. One of the composite manufacturing steps is to apply a temperature profile that should be determined specifically for the resin system. The temperature applications in the manufacturing processes mostly accelerate the flow of the resin and ensure the curing of the part, that forms the final solid state of the part. Effective density, specific heat capacity and conductivity properties for both resin and fiber can be initially defined and cannot be constant during process due to the increasing trend in the resin filled area, that's the reason to use effective material properties in General Heat Transfer equation. The used equation form in "Heat Transfer in Porous Media" can be seen in Equation [3.5].

$$d_z (\rho C_p)_{eff} \frac{\partial T}{\partial t} + d_z \rho C_p(\overline{u}, \nabla T) = d_z k_{eff} \nabla^2 T + q_0 + d_z Q$$
[3.5]

Where sub *eff* states effective material properties in computational domain, ρ density of air and resin seperately, C_p specific heat capacity, k conductivity of resin and fiber, d_z thickness of the domain, q_0 out of plane radiation or heat flux value, Q source term that mentioned in Equation [2.15], where specifies the exothermic heat source due to curing in the process.

3.4. Cure Kinetics Equations

In addition to the Heat Transfer in Porous Media module seen in the previous title, degree of cure analysis due to temperature profile was implemented corresponding to cure kinetics equation defined in the domain. The curing and viscosity equations that are solved in conjunction with the heat transfer equation, are numerically analyzed by using "Coefficient form of PDE" under "PDE Interfaces" in "Mathematics" module in Comsol Multiphysics® software. This interface gives user to specify the problem and let addition of equation, weak contributions, and constraints to modify main governing physics. The general form of PDE formulation can be seen in below,

$$e_a \frac{\partial^2 u}{\partial t^2} + d_a \frac{\partial u}{\partial t} - \nabla (c \nabla u + \alpha u - \gamma) + \beta \nabla u + \alpha u = f \qquad \text{in } \Omega \qquad [3.6]$$

$$n. (c\nabla u + \alpha u - \gamma) = g - qu + h^{T}\mu \qquad \text{on } \partial\Omega \qquad [3.7]$$
$$0 = R \qquad \text{on } \partial\Omega_{c} \qquad [3.8]$$
$$u = r \qquad \text{on } \partial\Omega_{d} \qquad [3.9]$$

Where Ω computational domain, $\partial \Omega$ domain boundary, *n* is outward normal vector on domain boundary. The main equation that the solution boundary specified, is Equation [3.6], the general expression Neumann boundary condition is Equation [3.7], Dirichlet boundary condition is Equation [3.8], and last equation set states special conditions in the main equation.

In finite element terminology, Neuman boundary conditions are called natural boundary conditions, but this condition does not occur in partial differential equations in a weak form. In the PDE interface, this is called flux or source because Neuman boundary conditions define a certain numerical value at that boundary. Dirichlet boundary conditions are called the basic boundary condition, these boundary conditions impose a limitation on the main domain. In the PDE interface, the Dirichlet boundary condition is the definition of the assigned variable in function form, in the Neuman boundary condition, this is a certain numerical value [36].



Conservative Flux

Figure 3.2. The name interpretation of main PDE equation

The solution of cure kinetics equation with these PDE module have been obtained with modifications of coefficient that explained in Figure 3.2 and named in Table 3.2. The damping coefficient is set to be 1, so that the left-hand side of PDE equation can be similar to cure kinetics equation. The source term for cure kinetics equations again is written as right hand side same equation. The mass, conservative flux, diffusion and absorption coefficient are set to be 0, so both sides of cure kinetics equation become exactly same. "Heat Transfer in Porous Media" module that is explained in above chapter, will be coupled with "Coefficient form of PDE" module. The degree of cure ($\frac{da}{dt}$) with total reaction heat (q_t) become source term in "Heat Transfer in Porous Media" module.

Symbol	Coefficient Name
e _a	The mass coefficient
d_a	The damping coefficient
С	The diffusion coefficient
α	The conservative flux convection coefficient
γ	The conservative flux source term
β	The convection coefficient
α	The absorption coefficient
f	The source term

Table 3.2. Coefficients of PDE equation in COMSOL Multiphysics ®

3.5. Consolidation with Arbitrary Lagrangian-Eularian Method (ALE)

Multiphysical modelling of VBO process also includes consolidation that the total volume of prepreg simultaneously changes due to vacuum bag pressure and fiber bed compaction stress during process. The change of volume during process can be modeled

with "Arbitrary Lagrangian-Eulerian" (ALE) module under "Moving Mesh", "Mathematics", respectively. This module provides to move solution meshes in time dependent studies, and also offer a numerical solution that can both remove major distortions and provide a correct solution using a kinematic description.

The Lagrangian and Eulerian are two mathematical explanations that describe motion in the meshes of computation domain. The Lagrangian formulation, usually used in structural mechanics problems, deals with modelling of anisotropic, solid materials that can solve deformation of material independent from current spatial orientation of anisotropic material. However, the Eulerian method does not have ability work with moving boundaries, that only can work with predefined mesh coordinate systems, so the problems that have time dependent deforming domain, cannot be handled with this formulation. The solution only can be found to remesh computation domain for each time iteration that makes Eulerian method unfavorable [36]. Hence, the ALE method that have been developed to suppress disadvantages of both method and highlight advantages of them, combines both method to allow moving boundaries with the mesh movement to contrary of material domain changes [36]. COMSOL Multiphysics' built-in function Moving Mesh (ale) is coupled with volumetric strain changes formulation (Equation [2.20]), will be defined as prescribed boundary velocity that the computational domain will deform in each time increment, which can be a function or a constant value.

3.6. The geometry of Solution Domain for Out of Autoclave prepregs

The impregnation resin through dry fiber in the prepreg is critically important, and also for evacuation of the air inside prepreg. Because of this reason, the type of fiber distribution in prepreg, for example, unidirectional, twill, weave etc, can be different, but important for the sake of manufacturing process. However, the initial fiber content, and the initial resin content of the prepreg is basically prepared in prepreg manufacturing lines. The resin film thickness value and the numbers of fibers in the tow governs that the initial resin and fiber content.

During the thesis, one standard prepreg system is chosen to be used, which is KOM12 low-temperature OoA prepreg. The initial parameters of the prepreg is given by the

manufacturer, KORDSA[®]. The optical microscope has been used to identify through thickness image of KOM12 prepreg in order to construct geometrical base for the modelling part.

First, the light microscopy images are obtained in order to observe the porous structure of prepreg, and then the resin film and the fiber parts are identified. The investigation for the tow inside prepreg is performed again with light microscopy. The resin film, and the fiber bed is clearly identified with light microscopy as well as the geometry of fiber tow (Figure 3.3, a). The detail geometries of prepreg is achieved with Micro-CT. The identification of resin films from both side and the fiber tow in middle, are measured as the resin film thickness is approximately 0.15 mm, the fiber content is about 0.35 mm in the middle (Figure 3.3, b). The simplified through thickness of prepreg in order to construct basis for the modelling section, has been achieved. During the thesis, this geometrical features for resin and dry fiber (Figure 3.3, c), will be used to interpret prepreg.

Light Microscopy





Figure 3.3. The goemtry determination procedure for KOM12 OoA prepregs, a) Light Microscopy images, b) Micro-CT image, c) simplified geometry for modelling

3.7. Boundary and Initial Conditions

The mathematical modelling of VBO process coupled with Multiphysics that are Darcy's flow, heat transfer and consolidation, aimed to find instantaneous porosity $\phi(t)$, degree of cure $(\frac{d\alpha}{dt})$. The nature of the VBO process requires to handle several physics that are explained and expressed in above titles. The Darcy Law (Equation [2.1]), General Heat Transfer (Equation [2.15]), and consolidation (Equation [2.19]) must be solved in order to achieve this multi-physical modelling of VBO process coupled with each physics. For the solution of equations, the material properties or parameters such that viscosity (μ), permeability (K), porosity (\emptyset), pressure (P), conductivity (k), density (ρ) etc., must be predefined, and releted with governing equations. The all parameters of multiphysical VBO process parameters and properties that are put into main equations, are given in Figure 2.1. The boundary and initial conditions must be defined in accordance with realistic representation of VBO composite manufacturing process. Since the problem are defined with 3 major governing equations in the form of differential equations. The boundary and initial conditions must be defined and that will be explained Darcy Law, Level Set equation, General Heat Transfer, and consolidation, respectively.

The numerical module required for the solution of Darcy's Law is available in Comsol Multiphysics. The use of this module is regulated for the VBO composite manufacturing process. In VBO process, the boundary conditions have been determined so that the maximum pressure difference is 1 [atm]. The initial pressure value is given from the top surface in the calculation area, atmospheric pressure, and the vacuum pressure difference is given from the air-filled area in the prepreg material (Figure 3.4). The boundary conditions providing fluid inlet and outlet into the calculation area have reached zero values and any fluid inlet and outlet except the amount of resin available, is prevented during the calculation, thus, this is not possible in the VBO process with prepreg materials.

In addition to the boundary conditions in Darcy's Law, material definitions, air resin density (ρ_{air}), viscosity values (μ), initial void value $\emptyset(t)$ and permeability tensor (K), should be defined. The resin density (ρ_{resin}) value was determined based on approximated literature experiments. Air density and viscosity values were determined to

be dependent on the stable operating range of the Level Set equation used in the flow front tracking. The first porosity value (\emptyset_o) , obtained experimentally varies in proportion to the fiber volume change as stated in the consolidation model equations $(1 - \emptyset(t) = v_o)$. The permeability tensor varies with the amount of fiber in the computation domain.



Figure 3.4. Boundary conditions for Darcy's Law

The resin flow due to the pressure difference in the computation domain, is calculated by Darcy Law, and the time dependent tracking of this flow is obtained with the Level Set equation. The Level Set equation performs a solution using the time-dependent change of the Level Set parameter (\emptyset) that was initially assigned. This change enables flow front tracking by calculating the volume average velocity differences between air and resin flow, starting from the initial interface of the liquids. Since initially there are only air and resin fluids on the prepreg, the level set parameter value (\emptyset) has been determined as the boundary conditions, 1 for resin and 0 for air, which varies from 0 to 1 depending on time. Since the volume average velocity of the resin flow is already found by Darcy Law, the regions where the level set parameter ($\emptyset = 1$) is changed with this value. In addition, assuming that there is no flow in all the external boundaries in the calculation domain and that the existing resin cannot flow out of the calculation area. As can be seen in Figure 3.5, where the boundary conditions are specified, the fluid outlet and inlet are defined for computational stability, and no resin increase occurs during the solution.



Figure 3.5. Boundary condition for Level Set Equation to flow front tracking

Level Set Method is an advanced method that is frequently used in fluid mechanics problems. The use of this method varies according to the type of problem and the material properties of the liquids used. There are studies in the literature using Level Set equation according to fluid density and viscosity ratios, that used in literature [16]. In our problem, the choice of parameters used in the solution of this equation is very important, since the density and viscosity ratios are very different from each other, because the resin and the viscosity whose time varies depending on the time. Reinitialization parameter (γ) and interface thickness parameter (ε_{ls}) values will be discussed in further chapter.

The resin in prepregs is exposed to both flow and curing throughout the VBO process. Temperature profile properties should ensure the resin to be cured. The resin also loses its viscosity as the temperature increases. Incorrect temperature profile applications here may cause voids that are not impregnated with resin in the VBO process. Void formation definitely affects the mechanical properties in the manufactured parts. For this reason, the temperature profile should be optimized according to the resin characteristic in the VBO process. The material properties required to perform special optimization studies for the resin system and the necessary boundary conditions (Figure 3.6) for observing the temperature distributions and the amount of exothermic heat generated during curing.



Figure 3.6. General Heat Transfer boundary conditions

The boundary conditions required for resin flow, heat transfer numerical solutions and required material properties, are presented above. Another physics required for multiphysical VBO process, is consolidation boundary conditions. the time-dependent calculation of thickness value change is performed with the ALE module in Comsol Multiphysics. Instantenous thickness change of prepreg is calculated with coupled Equations [2.17] and [2.20]. Linear volumetric strain rate is given as displacement in y axis of domain (Figure 3.7). The boundary conditions were determined in the calculation area assuming that the lowest limit is fixed and that the area can only change from the top limit.



Figure 3.7. Consolidation physics boundary conditions

As a result, the necessary boundary conditions and material properties for VBO process numerical analysis must be obtained for multiphysical modelling of VBO process with commercial OoA prepregs. In the light of the studies in the literature, the equations used in composite manufacturing processes are brought together for the VBO process. A completely related numerical model has been developed that will form the basis for the numerical solution and optimization studies of the VBO manufacturing process to be applied to the 1,2 and 4 layered prepreg systems. The developed model results will be shared in Chapter 5.

Chapter 4

OPTIMIZATION OF VACUUM BAG ONLY PROCESS

After explaining main governing physics of multiphysical VBO process, the completed model needs to be subjected to optimization study in order to minimize void content in final cured parts. The systematic directions in this thesis aims to deliver scalable, controllable and repeatable VBO process by receiving help from computational tools. After getting accurate and consistent model for multiphysical VBO process, the optimization study will start to find optimum process parameters such as compaction pressure, temperature profile (dwell time, ramp rate, initial and post cure temperature), consolidation time. The model can be run with the initial process parameters, and analyses void ratio in computational domain. Then, this initial void content of prepreg checked for target void content, which is defined under %1 void content in final cured parts as supposed to be used in aviation industry. The convergence of target void content in prepreg have been achieved by iterating new process parameters with decision maker Nelder-Mead algorithm. The flow chart that summarizes, and the iteration procedure the optimization part with the Nelder-Mead Algorithm in this thesis can be seen in Figure 4.1.

In order to get benefit from the developed multiphysical VBO process manufacturing model, the extension of the model with the optimization study can potentially help to find optimum process parameters due to multiphysical nature of the developed model, which is simultaneously calculated resin flow, heat transfer and consolidation physics. To explain Figure 4.1 flowchart, firstly, the model is started with the initial assigned parameters that is the recommended temperature profile parameters. The initial void content with this profile is obtained, and then, the difference between the target and the

numerical void content is compared. The determination to reestablish new process parameters by the Nelder-Mead algorithm is the next step for the VBO manufacturing optimization. The decision-making strategy in the Nelder-Mead algorithm will be explained in further sections. After the algorithm, the new process parameters have chosen to run model iteratively, until the target void content is achieved.



Figure 4.1. The optimization flow chart of developed model

4.1. Problem Statement

Mutliphysical VBO manufacturing modeling studies were obtained for 1, 2 and 8 layer prepreg systems. In numerical analysis models, prepreg material properties are integrated for the resin flow, the heat transfer and the consolidation physics that are calculated with the fully coupled manner. While moving to the optimization step, the parameters used for VBO manufacturing modeling should be reviewed and the effective process parameters should be determined. Since the VBO process is governed by multiphysiscs, the governing parameters that significantly affect the whole process, must be chosen wisely. The consolidation time, the temperature profile, and the compaction pressure are the main effective parameter. Apart from these parameters, the temperature profile parameters are already affects all these three physics, so the parameter that will be used in the optimization study have chosen to be the temperature profile parameters. The initial and post cure temperature, the dwell time and the ramp rate are determined to be used in the context of the optimization. The classical temperature profile representation that is used for VBO manufacturing, can be seen in Figure 4.2.



Figure 4.2. The classical temperature profile during VBO manufacturing and the representations of the optimization parameters on the temperature profile

The parameters in the temperature profile are determined as the initial temperature, the initial cure and post cure temperature, the dwell time, and the temperature ramp rate (Figure 4.2). The applied optimization algorithm will find the optimum temperature profile parameters with the result of the changes in these parameters in the specified ranges that are predefined. In the flow chart shown in Figure 4.1,the VBO production process is run with the determined process parameters. According to this solution, Nelder-Mead algorithm decides with which parameters to create a new solution in the next numerical solution. It controls the amount of space we have defined in the algorithm. This control works until the target amount of filled area is reached. Detailed Nelder-Mead simplex algorithm will be explained.

4.2. Nelder-Mead Algorithm

In order to evaluate algorithm working principle, the mathematical description of Nelder-Mead simplex algorithm should be explained. The method is a simplex based method which defined n+1 corner point in the n-space S as convex body. However, it does not need any gradient value [40]. The values of objective function evaluated with dependent variables of these parameters in the n+1 simplex corner point. These values continue until the target function value is provided to maximize / minimize the function values at the corner points within the specified parameter limits. The path to determine new parameters is evaluated in the algorithm with several actions.



Figure 4.3. The geometrical description of the Nelder-Mead algorithm [41]

Nelder-Mead algorithm decision making mechanism is shown in Figure 4.3. The geometric expressions are the simplexes that are consist of corner points. Each corner of the triangle-shaped simplex coincides with one parameter, and it performs reflection, shrinkage, expansion and contraction (Figure 4.3) according to the objective function results. At the center of the triangles are the target objective function values , whichever parameter value is closer to that value, the Nelder-Mead algorithm determines movement of the simplex as shrinkage, expansion, contraction or reflection. Thus, the objective function value is maximized or minimized. This algorithm is defined in the Optimization module of the Comsol program and can be operated with other physics.

As the purposes of the thesis to model multiphysical nature of the VBO process, the integration of the model studies with the optimization study has to be understood. The achievements with the model part of this thesis explained in the result section, also the aim to construct the optimization study explained. The assigned initial model parameters for each of parameters mentioned in Figure 4.2 is solved for predetermined intervals first, while the other parameters are constants. Hence, the construction of first simplex is completed, after that the Nelder-Mead algorithm determine the next steps values by

comparing the objective function values. The working cycle for the algorithm with the integration of the multiphysical VBO manufacturing model can be seen in Figure 4.4.



Figure 4.4. The flowchart of the integration of the model with the Nelder-Mead algorithm

4.2.1. Nelder-Mead Algorithm Implementation

Void ratio, radius, and distribution highly depends on the process parameters such as magnitude of vacuum pressure, temperature profile parameters (ramp rate, dwell time, initial cure temperature etc.), consolidation time [29]. After VBO process completed, the effect of process conditions with relation of material properties for both resin system and

fiber architecture significantly govern the void characteristics, in addition to void initiation mechanism. The determination of right processing conditions in VBO process is vital for reduction of void in final cured parts. The reason to use optimization study in integrated VBO modelling is to identify these process condition parameters. The solution for optimization of multiphysical VBO process modelling is calculated with the Nelder-Mead Simplex algorithm. It is a direct-search method in the sense that it evaluates the objective function at a finite number of points in computational domain per each different parameter iteration. According to increasing or decreasing of objective function, the algorithm decides to converge target objective function value.

Type of algorithm	Name of Algorithm
Derivative free optimization options	Coordinate Search
	• Monte Carlo
	• Nelder-Mead
	• BOBYQA
	• COBYLA
	• SNOPT
Gradient base optimization options	• MMA
	• Levenberg-Marquardt

Table 4.1.Optimization types and options in COMSOL Multiphysics ®

The optimization in Comsol Multiphysics[®] is a part of additional solution type under "Mathematics", "Optimization and Sensitivity" and "Optimization" module that can be added just like other main physics equations. On the other hand, the optimization module can be performed as an extension of "Study" in Comsol Multiphysics[®] as well. The optimization solver types in Comsol Multiphysics[®] based on derivative free or gradient base problems can be found in Table 4.1. The Nelder-Mead algorithm that selected to achieve optimum process conditions, is built in function that the user can specify maximization or minimization of objective function in the limits of optimality tolerances, and maximum number of model evaluations. The initial parameters also have to be in definite ranges, also limited range of constraints. The decreasing or increasing in these parameters determined according to the penalty method.

4.2.2 Nelder-Mead Algorithm Case Study

Since Comsol Multiphysics® software is used for numerical analysis, a case study has been done in order to be a preliminary study and to test the Nelder-Mead algorithm, which is a module defined in the program. Firstly, preliminary studies have been carried out to apply the algorithm to the integrated VBO process model. In these preliminary studies, the isothermal, constant viscosity resin flow in a porous medium was aimed to solved with the Nelder-Mead algorithm. For this purpose, Darcy's Law and Level Set equations have been solved. The problem was defined as 75% resin filling rate for the predefined domain in this example study. The aim of this study to just include Darcy's Law and Level Set Equation is to reduce the calculation time in simulation and optimization stages. The geometry of the problem has been chosen to be 1-layer prepregs geometrical properties. Thus, after this study, the adaptation of the algorithm was performed and the simplex formation and progression mechanisms in Figure 4.3 were verified. With this example study problem, it was aimed to calculate how long it takes, the targeted 75% fill ratio would be achieved. The algorithm objective function is the area filled with resin, and the algorithm search for the time parameter in the unit of seconds. The flow chart, which is the summary of this study, is shown in Figure 4.5.



Figure 4.5. Example problem flowchart for the Nelder-Mead algorithm

The problem defined in this case study solves the resin flow through porous media together with the consolidation physics. The vacuum pressure defined through porous media is provided to initiate to resin flow in the domain, and the flow front is tracked with the Level Set equation. In consolidation, geometry was reduced at constant speed from the upper limit of geometry. The objective function has been defined as the target area (%75) filled with the resin. For the ease of the computational cost of the problem, the heat transfer and curing properties are not included in this model.

The problem was first run for 400 seconds to obtain the initial fill ratio of 0.515873 (initial data point). Then, the algorithm determines the new time values by adding 5 seconds for each iteration, to check objective function, and continues for 405, 410 and 415 seconds. The algorithm calculates the filling times in order to reach objective function values (Figure 4.6). The algorithm was able to determine that 75% of the area was filled in 700 seconds after 32 steps. As it can be seen in Figure 4.6, because much more filling than the desired 75% filled ratio was realized in the 15th trial, the last decision was shrinking, and the filled rate was defined between 80% and 68%. Later, it approached the value of 75% by oscillating between these time values. To sum up, the working principle of Nelder-Mead algorithm in Comsol Multiphysics® software was understood with this study, and the experiences we gained from this problem were used in determining the effective parameters and determining the first parameter values, which are used for the Nelder-Mead algorithm in Comsol Multiphysics®.



Figure 4.6. The time decided by the Nelder-Mead algorithm for this example problems (left), the change of the objective function depending on the number of steps (right)

4.3. Vacuum Bag Only process optimization for 1-Layer prepreg

After the implementation of Nelder-Mead algorithm in Comsol software with the previous example study, it should be used for the optimization of the process parameters of the algorithm with the integrated VBO manufactuing process model. Within the scope of this thesis, the pressure, the temperature profile and the consolidation time are defined as process parameters. Since the application of the temperature profile in the VBO process has an integrated effect on the resin flow, curing degree and consolidation physics, the parameters in the temperature profile are determined to be used in the optimization algorithm at this stage. An example temperature profile of a VBO process is presented in Figure 4.2. In this study, at a constant initial temperature, i) the ramp rate, ii) the initial cure temperature, iii) the dwell time and iv) the post cure temperature values were optimized for the minimum void ratio, maximum filled area. In addition, the minimum void ratio in this study was determined as 12% for this preliminary study. Therefore, from the results here, the required 1% void rate for the aviation standards mentioned in our project is not expected.

The optimization algorithm to be applied will find the optimum temperature profile parameters as a result of the changes of these parameters in the specified intervals. In the flow chart shown in Figure 4.4, the model of multiphysical VBO manufacturing process is run with the determined process parameters. According to this solution, Nelder-Mead algorithm decides with which parameters to create a new solution in the next numerical solution. It controls the void ratio as the objective function. This control works until the target amount of area is reached.

The purpose and application method of the optimization algorithm have been explained and the method described has been applied for the 1-layer prepreg system. This application was run with Nelder-Mead algorithm, with the parameters in the temperature profile at certain intervals and the initial step numbers are predefined. This algorithm works depending on the starting parameters, and careful selection of the starting parameters is critical to success. The initial values of the working methodology proposed in the project are shared in this section. The initial temperature profile parameters are given in Table 4.2.

Parameters	Initial values
Initial cure temperature	60 °C
Post cure temperature	100 °C
Ramp rate	1 °C/ <i>dk</i>
Dwell Time	40 <i>dk</i>

Table 4.2. The initial temperature profile parameters used in this study

As a result of the application of the optimization algorithm for the numerical analysis of the Out of Autoclave manufacturing of the 1-layer prepreg system with Vacuum bagging (VBO) method, the last convergence values of the parameters are given in Table 4.3, and the development of these values as a result of about 100 iterations is shown in Figure 4.7. As it can be understood from the graph that the parameters converge, the use of Nelder-Mead algorithm progresses and gives results for the temperature profile parameters.

Parameters	Initial values
Initial cure temperature	85.2 °C
Post cure temperature	137.98 °C
Ramp rate	3.2926 °C/dk
Dwell Time	79.9 dk

 Table 4.3. The last values of the temperature profile parameters found with the Nelder

 Mead algorithm

According to Figure 4.7, the results to be obtained from this study can be evaluated for each parameter. The change in the initial cure temperature value, which is the first parameter of the temperature profile, changes the objective function more than the other parameters (10-20 iterations) that is also physically true as well. The initial cure temperature increases the resin impregnation in the prepreg while reducing the resin viscosity. The ramp rate increase does not affect the amount of void but plays an active role for the degree of cure of the part (around 50 repetitions) [23]. In the interval where the dwell time changed, the objective function changed significantly (between 40-60 repetitions). The change in waiting time is effective in resin impregnation as described in the literature [42].

The development of the objective function with the Nelder-Mead algorithm is presented in Figure 4.8. The number of iterations (x-axis) indicates the number of runs the multiphysical VBO manufacturing process model of 1- layer prepreg. The resin filling ratio of 62% obtained from the result of the first model reaches 80% in the number of 50 iterations and 88% after iterations of 100. The result obtained here is that the optimization algorithm specified for multiphysical VBO manufacturing process can be applied to the temperature profile parameters to obtain void reduced parts.



Figure 4.7. The converging values of defined parameters in Nelder-Mead Algorithm



Figure 4.8. Change of resin fill ratio with each iteration of Nelder-Mead algorithm solution of 1-layer prepreg system

Chapter 5

RESULTS AND DISCUSSION

In this chapter, the multiphysical model development will be shown step by step with the mathematical formulations in Chapter 2. The result of the implementation of these formulations with Comsol Multiphysics® in Chapter 3 will be shared in order to ensure that multiphysical VBO manufacturing process is achieved. First, the integration of the physics is obtained, and then the multiphysical VBO manufacturing process model integrated with the resin flow, heat transfer and consolidation is implemented for the 1, 2 and 4 layer of OoA prepregs. The parametric study and the optimization with temperature profile parameters is presented and interpreted by comparison of the literature studies.

5.1. Integrated Vacuum Bag Only Process Modeling Studies

The aim in developing numerical analysis of VBO manufacturing process is to obtain realistic void ratio by doing numerical analysis in computer environment. The purposes to attain void ratio with the developed model is to construct base for the optimization of VBO manufacturing process with the integrated multiphysics. In this section, the model development procedure with the basics of composite manufacturing process modelling is explained, and the multiphysical model of VBO process is completed in 8 steps by sharing the result of each steps. The roadmap for this section can be seen in Figure 5.1.


Figure 5.1. Flowchart of integration of physics with Comsol Multiphysics®

5.1.1. Darcy's Law Adaptation

The modelling of porous structure in VBO prepreg systems is encouraged to formulated with Darcy's Law that has been mentioned in Chapter 2, and explanation of implementation in Comsol Multiphysics® Chapter 3. The effective parameter analysis in 2D through thickness VBO prepreg is analyzed. The Darcy's velocity in porous domain is initiated mainly driven by pressure difference in addition to viscosity of resin, and permeability of fiber bundles. However, the velocity that has been found with Darcy Law, is a superficial velocity of resin. Due to consolidation that volumetric change of computational domain, the velocity has to increase proportional to porosity of prepreg, so

Darcy's velocity, superficial velocity, should be converted to the actual velocity of prepreg by multiplying with instantaneous porosity.

The geometry to conduct analysis has been chosen to represent through thickness the small portion of the prepreg 0.5 mm in the height and 0.5 mm in the width. Prepreg is assumed to be impregnated with resin about %30 in area and has constant resin viscosity. The prepreg with 0.5 porosity is subjected to 1 (atm) vacuum pressure to initiate the velocity of resin with the isotropic permeability. Applied boundary conditions for Darcy's Law is shown in Figure 5.2. The initial material properties for both fiber and resin are given in Table 5.1.



Figure 5.2. 2D Darcy Law boundary conditions

The aim for this study to ensure that the resin velocity can be initiated with the VBO process conditions by Darcy's Law, to detect the pressure distribution (Figure 5.3, a) in vacuum port side of the prepreg. The velocity field in through thickness direction can easily be created with applied processing conditions (Figure 5.3, b).

Material Properties	Values
Resin density	1180 (kg/m^3)
Resin viscosity	0.1 (Pa.s)
Porosity	0.5 (1)
Permeability	$1E-10(m^2)$
Vacuum Pressure	1 (atm)

Table 5.1. Material properties table for simple Darcy Law solution



Figure 5.3. 2D Darcy Law solution in example geometry for a) pressure distribution, b) Darcy velocity distribution

5.1.2. Darcy's Law coupled with Level Set Equation

The time dependent resin flow front location analysis can offer to detect resin impregnation rate during VBO process, because the initial resin quantity and the location of it, in through thickness of prepreg can become a known parameter. The velocity of the fluid, the resin, have been calculated with the Darcy's Law equation that governed by the pressure gradient, and dependent to resin viscosity, density and fiber permeability of porous domain. The parameters that are required to know for porous media flow, Darcy's Law, have been used to detect instantaneous flow front of resin coupled with Level Set Equation. The velocity occurred in porous domain is given as an input to Level Set Equation, so that the location of resin flow front dependent with the instant velocity of resin can be tracked by this coupling scheme. The implementation of this coupling scheme has been tested with a case study, to observe the flow front progression of resin in porous domain. The boundary condition for Level Set equation has been mentioned under Chapter 3.

Material Properties	Values
Resin density	1180 (kg/m^3)
Resin viscosity	10 (Pa.s)
Porosity	0.5 (1)
Permeability	$1E-12(m^2)$
Vacuum Pressure	0.01 (atm)

Table 5.2. Defined parameters required to solve Level Set Equation

The Darcy Law coupled with Level Set equation helps to find instant flow front position in solution domain. The velocity initiated in Darcy Law is used as convective velocity field in Level Set equation. This velocity field has been used in Level Set equation (Equation [3.2]), to track each level set parameter, which are between 0 and 1, directed accordingly. The model shown in this section aims to prove mathematically the tracing of flow front position, is possible, if the velocity field is known. The example model in Figure 5.4, presents the propagation of a fluid under vacuum pressure. However, this example model studied to get experience on coupling of Darcy Law and Level Set equation.

This case study is conducted on the resin and fiber properties presented in Table 5.2. the domain is again assumed to be under VBO manufacturing conditions, but the magnitude of the vacuum hold is assumed to be lesser than the actual atmospheric vacuum (1 atm), since the domain is small compared to the actual prepreg sheet. Geometrical feature of the prepreg is 0.5 mm to 0.5 mm through thickness prepreg. The coupling of Darcy equation with Level Set is crucial to get time dependent resin flow front position. For this reason, reinitialization and interface thickness parameters should be determined based on the Darcy velocity and the maximum mesh size length [43], for this reason, the properties shown in Table 5.1 and Table 5.2 are different because of the integration that has to be accomplished.

Level Set Parameters	Value
Reinitialization parameter	1E-7 ($m/_{S}$)
Parameter controlling interface thickness	1.75E-5 (<i>m</i>)

Table 5.3. Defined parameters required to solve Level Set Equation

As can be seen in Figure 5.4, the velocity initiated with Darcy Law has been successfully tracked by the Level Set equation. Since the model does not have temperature dependent properties, the constant velocity is tracked with the time range of 1000 seconds. The level set parameters for Darcy's Law properties (Table 5.2) can be integrated each other with the parameters shown in Table 5.3.



Figure 5.4. The time dependent flow front positions for a fluid through porous media under vacuum pressure

5.1.3. Consolidation Physics with Arbitrary Lagrangian-Eularian Equation

The Arbitrary Lagrangian Eulerian (ALE) method used to interpret the volumetric change of solution domain in VBO prepreg systems. The consolidation in prepreg causes to decrease in through thickness direction. The ALE boundary conditions to correctly interpret consolidation physics during VBO process consist of several parameter such as compaction pressure, fiber volume fraction, evacuation of air etc. The mathematical description of these physics, the formulations, have been identified in Chapter 2. The volumetric change in through thickness direction coupled with Henry's Law has been used in 1, 2 and 4 layers of multiphysical VBO manufacturing process modelling. However, the results shown in this section is only aimed to discover ALE module. The predefined velocity value at the top boundary is applied into the solution domain. Then, the fluid flow through porous domain have been followed with the Level Set equation that has been mentioned in previous section. The developed model for the flow front analysis has been used for this model, the properties (Table 5.2) and level set parameters (Table 5.1). In addition, the consolidation velocity has been predetermined (1e-7 m/s) from the top of the prepreg. The boundary conditions for ALE module is applied as same as explained in Chapter 3. As a conclusion of this case study, the analysis of flow front under consolidated domain can be achievable and the consolidation behavior in VBO process coupled with Darcy's Law and Level Set can be modeled with ALE module in Comsol Multiphysics® as given in Figure 5.5.



Figure 5.5. Time dependent consolidation effect on throught thickness of prepreg solved with ALE

However, Level Set function is used to interpret the density and the viscosity of air and resin as a function of level set parameter. The change of density and viscosity in solution domain effects the computation for resin flow, heat transfer and, thus consolidation. For this reason, viscosity and density computation as a function of level set parameter (phils) is performed within Level Set Method calculations, which is expressed in Equation [3.3] and [3.3]. The coupling with Level Set equation of viscosity and density equation as Comsol Multiphysics[®] implementation can be seen in Figure 5.6 and Figure 5.6.



Figure 5.6. The level set equation solution for the density Equation [3.3] as initial and final solution time (0s-1000s)

Time=1000 s Dynamic viscosity (Pa*s) Time=0 s Dynamic viscosity (Pa*s)



Figure 5.7. The level set equation solution for the viscosity Equation [3.3] as initial and final solution time (0s-1000s)

5.1.4. Heat Transfer in Vacuum Bag Only coupled with Cure Kinetics and Viscosity Models

Heat transfer application in composite manufacturing process have been described in Chapter 2 and explained the implementation through Comsol Multiphysics® software in Chapter 3. The cure kinetics, and the viscosity models for specific resin systems can significantly affect the result of process in terms of impregnation rate, degree of cure etc. However, the viscosity model should be applicable in a situation, where the degree of cure and the viscosity coupled each other. During the multiphysical modelling of VBO process, the increase in curing degree also supplies increase in the viscosity. The coupling of both the viscosity (Equation [2.24]) and the degree of cure equations (Equation [2.22]), on General Heat Transfer equation (Equation [2.15]) eventually the results of implementation case, have been presented in this section.

The case study is conducted on the realistic prepreg with the geometry of 0.5 mm x 0.5 mm that assumed to have resin film in both sides different from previous geometries. The thermal properties for the resin and the fiber can be seen in Table 5.4. In order to analysis thermal properties of the prepreg, the temperature profile for VBO manufacturing is chosen to be recommended profile by the manufacturer company KORDSA®. The recommended temperature profile during the thesis will implicate Figure 5.8 which has 85 °C initial cure temperature, 120 °C post cure temperature, 2 °C/*min* ramp rate with 60 *min* dwell time for each temperature steps [44]. Applied boundary conditions arranged to refer oven curing, which the temperature profile applied on 4 sides.

Material Properties	Values
Resin thermal conductivity	0.2 (W/(m.K))
Resin density	1180 (kg/m^3)
Resin Heat capacity	850 (J/(kg.K))
Fiber volume fraction	0.5 (1)
Fiber Thermal conductivity	3.2 (W/(m.K))
Fiber density	$1850 (kg/m^3)$
Fiber Heat capacity	1200 (J/(kg.K))

Table 5.4. Thermal properties of resin and fiber for Heat Transfer equation

The cure kinetics and the viscosity equations mentioned in Chapter 2, has developed for the resin system used in KOM12 prepreg [44], the parameters for these equation provides the degree of cure in specific temperature ranges that can be integrated with heat transfer equation. These parameters will be conducted for further models, and the parameters for cure kinetics in Table 5.5 and viscosity in Table 5.6.

Cure Kinetics Model Parameters	Values
A_1	$1.84 \times 10^{10} s^{-1}$
E_{1}	$94.301 \times 10^{3} J/mol$
A_2	$4.87 \times 10^8 s^{-1}$
E_2	$78.318 \times 10^{3} J/mol$
m_1	0.671
m_2	1.486
n_1	13.025
n_2	2.806
D	23.97
$\alpha_{\rm C0}$	-0.712
α _{CT}	$4.43 \times 10^{-3} \circ K^{-1}$

Table 5.5 The parameters used for the cure kinetics model

Table 5.6 The parameters used for the viscosity model

Viscosity Model Parameters	Values
A ₁	$6.54 \times 10^{-12} \mathrm{s}^{-1}$
Ε _{μ1}	81×10^3 J/mol
A ₂	$1 \times 10^{-30} \text{ s}^{-1}$
Ε _{μ2}	197×10^3 J/mol
А	19.78
В	-5.94
С	-29.2
α_{gel}	0.61



Figure 5.8. Recomended temperature profile for KOM-12 OoA prepreg system by KORDSA®

Initially, the prepregs started with the room temperature so that the viscosity in room temperature is higher. While the temperature increases within the profile, the viscosity of the resin started to decrease as expected from a resin system. The behavior of the viscosity compared to degree of cure is that the increase in the degree of cure, also rises the viscosity in the prepreg [6]. The volume averaged viscosity and the cure kinetics evolution of the prepreg with the recommended temperature profile is given in Figure 5.9.

The degree of curing and the total amount of heat released due to increase in degree of cure is reasonable according to source term of Equation [2.22]. To compare with the degree of the cure, the total heat has similar trend (Figure 5.10) with the degree of cure which is compatible with the literature [27],[30], [12]. In literature [6], the characteristic of the resin system is shown with comparison of the change of degree of cure with respect to cure rate as shown in (Figure 5.11). However, the result for the heat generation is more reasonable with cure rate graph. Because of the fact that the source term in heat transfer equation (Equation [2.15]) consists of total reaction heat of resin and the cure rate, so multiplication of these parameters at higher degree of cure can give maximum of 340 W/m^3 , which can be seen in Figure 5.10.



Figure 5.9. The viscosity (blue) and the degree of cure (green) change during VBO process



Figure 5.10. Exothermic heat generation (blue) graph during the degree of cure increasing (green)



Figure 5.11. The cure rate dependent with degree of cure during process for used resin system

5.1.5. Multiphysical VBO process modelling without consolidation

Darcy Law, the flow front tracking with Level Set equation, consolidation physics with ALE, heat transfer equation for cure kinetics and viscosity models, is intentionally presented one by one in order to understand the development of multiphysical modelling of VBO manufacturing process. Firstly, the multiphysical VBO process modelling, which includes Darcy Law, Level Set Equation, Heat Transfer with the cure kinetics and the viscosity models, have been studied without consolidation physics in order to prevent convergence issues, because consolidation physics with ALE module changes simultaneously mesh structure in solution domain. Due to change in mesh structure, the Level Set Equation does not convergence is that the level set equation parameters such as the initial interface thickness and the reinitialization must be rearranged. Another reason to study multiphysical model of VBO process is to observe the void initiation without the change in prepreg volume.

The computational domain and the boundary conditions for Darcy Law, Level Set equation, and Heat Transfer is applied as same as previous sections. The parameters for

the cure kinetics and the viscosity models is applied similar and expected to be same in mentioned sections. However, the focus of the thesis is defined on the instantaneous void analysis of VBO manufacturing. The parameter to evaluate multiphysical VBO process modeling is determined as the void analysis. The initial resin impregnated area and the dry fiber (the un-impregnated) is predefined in the domain, as the time goes by, the impregnated area will increase. The resin flow front with Level Set equation enables to detect the total impregnated area due to level set parameter assigned for both, resin and air. If the resin position is traceable in initial computation domain, one can simply calculate the change of the time dependent resin area (\emptyset_t) by integrating the level set parameter assigned for the resin (phils=0). The surface integral of the resin impregnated area (Equation [5.1]) and the time dependent change of this area (Equation [5.2]) can be seen below.

$$\iint_{0}^{h} (phils = 0) dx dy = \emptyset_{0}$$
[5.1]

$$\int_{0}^{t_{final}} \phi_0 dt = \phi_t$$
[5.2]

As soon as the temperature profile applied on prepreg, the viscosity of the resin starts to reduce so that the resin impregnated area increases. The resin flow front both top and bottom sides creates air evacuation channels that lets to escape the air between fibers in the direction of vacuum applied surface. Eventually, the closing in air evacuation channels correspond to the voids in the domain (Figure 5.12). The instant ratio of resin impregnated area to dry fiber area, void ratio, will be given in next section as comparison with consolidated solution domain.



Figure 5.12. The resin flow front evolution of multiphysical modelling of 1-layer of VBO prepreg without consolidation physics

5.1.6. Void Analysis of 1-Layer Multi Physical Modelling of VBO process

In this section of the thesis, the result of multiphysical VBO composite manufacturing process have been shown for 2D through thickness 1 layer of UD prepreg system. The un-consolidated solution domain results have been obtained. The comparison of un-consolidated solution domain and consolidated solution domain for multiphysical 1-layer VBO manufacturing will be presented. The difference between un-consolidated and consolidated domain for the void analysis is clearly exposed with results obtained in this section. The boundary conditions and the geometry are similar with un-consolidated study presented in previous section. The time dependent evolution of resin impregnation can be seen in Figure 5.13.

The effect of consolidation on the void initiation mechanism between un-consolidated and consolidated cases can be easily distinguished. The air evacuation channels in Figure 5.12 is approximately closed after 4000 second, but the closing of channels in Figure 5.13 starts before 4000 seconds. To explain this difference, the consolidation in VBO process exhibits earlier closing in air evacuation channels due to change in decreasing of thickness. However, the comparison of resin impregnation for both unconsolidated and consolidated solution domains also exhibits that the consolidated domain shows higher impregnated area so that lesser void content during VBO manufacturing. The consolidated domain is filled with resin about % 95 percent, while the un-consolidated domain is % 91.5 resin content after manufacturing cycle (Figure 5.14).



Figure 5.13. The resin flow front evolution of multiphysical modelling of 1-layer of VBO prepreg with consolidation



Figure 5.14. The comparison of resin impregnated area development during VBO process for the models with

Prepreg layer thickness change decreases in direct proportion with the evacuation of air in the prepreg. If there is an obstacle that prevents air evacuation at the edge of the prepregs during the VBO manufacturing process, such as silicon bands, the air that cannot escape, causes a higher void ratio in the prepreg. The important practical manufacturing consideration is that the prepreg should not be surrounded with any material that blocks the air evacuation during manufacturing. The consolidated solution domain effect on ALE module into the mesh structure can be seen in Figure 5.15.



Figure 5.15. The time dependent thickness change with regards to mesh movements provided by ALE module for 1-layer VBO manufacturing process

5.1.7. Void Analysis of 2-Layer Multi Physical Modelling of VBO process

1-layer VBO manufacturing process has been successfully implemented in virtual environment. This developed numerical modeling procedure was also applied for the manufacturing of 2-layer VBO that the results will be shared in this section. The boundary conditions and the equations are assumed to be valid for 2-layer multiphysical VBO manufacturing process modeling.

As it can be understood from the flow front tracking analysis results (Figure 5.16) for 2layer prepregs, that the void formation mechanism in 2-layer prepreg is similar to the 1layer prepreg results. The air evacuation channel formations tend towards the vacuum boundary conditions surfaces and progress over time. The development of air evacuation channels and the formation of voids in 2-layer is started later than 1-layer solution. After dry fiber entrapped with resin that creates closed surface, the filling time for these voids have more resistant to fill, which this inference can be seen from both 1-layer and 2-layer of multiphysical VBO process modelling.



Figure 5.16. The resin flow front evolution of multiphysical modelling of 2-layer of VBO prepreg

4.1.8. Void Analysis of 4-Layer Multi Physical Modelling of VBO process

After the numerical void analysis of VBO manufacturing process with 1 and 2 layers prepregs, performance evaluation for multilayered prepreg manufactured with VBO process is aimed to be shared in this section. Since the thickness values of the parts used in the aviation industry often require multi-layer manufacturing, for this reason, 4-layer VBO manufacturing is analyzed. The comparison with 1 and 2-layer VBO manufacturing model results will be presented in further sections. As shared in previous multiphysical VBO manufacturing results for 1 and 2 layers, the geometry for 4 layers is quadrupled in the length, and the boundary conditions has been kept same.

The resin flow front evolution of 4 layers multiphysical VBO manufacturing process is presented in Figure 5.17. After 2000 seconds, the air evacuation channels are closed, and the voids are started to be formed until end of the process. In 1- and 2-layer void formations, 1-layer solution showed that the closing of air evacuation channels are closed earlier than 2-layer solution. However, this behavior for 4 layers solution shows similar to 1-layer solution, it tends to close earlier compared to 2-layer solution. The reason for that 4 layers solution has higher volumetric strain rate because of the initial thickness of the prepreg is higher. On the other hand, the closing of air evacuation channels in 2-layers solution is more likely to be dominated by the resin flow, but the air evacuation channel forming in 4-layers solution is appeared to be due to higher consolidation. Furthermore, the comparison of the void ratios of 1,2- and 4-layers solutions will be given in next section. The multiphysical assessment of the developed model by sharing the effective parameters of individual physics also will be shared for these 3 models.

As a conclusion, the multiphysical VBO process modelling by integration of resin flow, heat transfer and consolidation equations, has been explained step by step. The void formation analysis has been chosen to present for the multiphysical assessment parameter. The initial results are given to visualize the resin flow in through thickness of prepreg. To get benefit from developed model, the process can be subjected to parametric studies and also process optimization studies.



Figure 5.17. The resin flow front evolution of multiphysical modelling of 4-layer of VBO prepreg

5.2. Integration Assessments for the void comparison

Development procedure of the multiphysical VBO manufacturing process has been described and resin flow front analysis for 1-, 2- and 4-layers prepreg is shared on preliminary results as void analysis. However, VBO process includes several different physics which are needed to be coupled with each other. The coupling scheme for these physics are also explained in Chapter 2. In this section of thesis, the effective parameters for each physics is presented in a way that the comparison of 1-, 2- and 4-layers solutions. The results that will be shown in this part, are aimed to present the multiphysical achievement obtained with the multiphysical VBO process modelling for 1,2 and 4 layers prepregs.

The resin flow is modeled with Darcy's Law that needs several parameters for both fluid and the porous domain. The domain porosity, and permeability are two of the important properties for the flow through porous media. Permeability of fibers is calculated with Kozeny-Carman relation (Equation [2.21]) and the porosity is calculated by Equation [2.17] with coupling of Equation [2.17] and [2.17]. Henry's Law coupled with the volumetric strain rate change that causes to change in porosity as well. Hence, the porosity change effects resin velocity as well as the consolidation in computation domain, so that the result for the porosity change is important parameter to evaluate the multiphysical modelling for VBO process modelling. The permeability of the domain is affected with fiber volume fraction, which is inversely proportional to porosity, likewise, related with the consolidation. Due to these reasons, the resin flow assessment for the multiphysical perspective, permeability versus fiber volume fraction will be evaluated.

Comsol Physics Name	Symbol	Value
Darcy's Law	$ ho_{resin}$	1850 (k g/m^3)
	$ ho_{air}$	18.5 (k g/m^3)
	$ ho_{effective}$	1850*(phils)+18.5*(1-phils)
	μ_{resin}	Visco ($Pa * s$)
	μ_{air}	100 (<i>Pa</i> * <i>s</i>)
	$\mu_{effective}$	Visco*phils+(100)*(1-phils)
	ϕ_p	0.626-por_del
	К	$1E-13^*((\in_p)^3/(\in_p)^2)$
Level Set Equation	γ	6*1e-5 (<i>m/s</i>)
	ϵ_{ls}	2*1e-5 (<i>m</i>)
Heat Transfer	k _{resin}	0.19 (W/mK)
	k_{fiber}	1.5 (W/mK)
	$C_{p-fiber}$	890 (kg/m ³)
	$C_{p-resin}$	1260 (kg/m ³)
	$Q_{reaction}$	340 (J/g)

Table 5.7. Defined parameters for numerical simulations by physics, level set parameters can vary for 1-,2- and 4- layer configurations, and some parameters written in Comsol Multiphysics® software language The heat transfer over the prepreg is calculated for the degree of cure and viscosity properties of resin system. The heated domain temperature distribution is directly effective during the curing of the prepreg, which the resin solidifies, also, the viscosity of resin that will increase the velocity of the resin through porous media. Therefore, the thermal properties of the developed models will be evaluated based on the temperature distribution that is calculated by the heat transfer equation (Equation [2.15]). The consolidation behavior of the models will be evaluated based on the total thickness change of the prepregs during VBO process. Since the model thickness are initially different from each other, for this reason, the change of the thickness as percentage of initial thickness is chosen to be compared for 1,2 and 4 layers of VBO process models.

The developed model parameters to run simulations for 1,2 and 4 layers of multiphysical VBO process modelling has been shared as a summation of the model runs. The properties written to interpret the mathematics for VBO process modelling, which is mentioned in Chapter 2. In Table 5.7, the used Comsol built-in function names with the mathematical symbols are presented in written forms of values.

Viscous resin progression depends on several parameters. Among these parameters, viscosity (Equation [2.24]) is computed as coupling of cure kinetics equation (Equation [2.22]). Assessment of resin flow parameter for integrated VBO model, as often seen in literature [11],[12], is chosen permeability change with respect to fiber volume fraction (Equation [2.21]). Permeability is decreased for increasing of fiber volume fraction during impregnation of prepregs. The described resin flow behavior for 1, 2 and 4 layers of prepreg, can be seen in Figure 5.18.



Figure 5.18. Permeability change with respect to fiber volume fraction for 1, 2 and 4 layers prepregs durin the multiphysical VBO process modelling

The coupling of resin flow to consolidation and cure kinetics, viscosity equations are shown an example of successful implementation of VBO process for composite manufacturing process design. Numerical tests for 1-, 2- and 4-layers prepreg subjected to VBO manufacturing have been run over time dependent temperature cycle to obtain each physics outcomes with constant number of free quad type mesh per layers. The standard geometrical dimensions for each prepreg layers are selected as 0.5 *mm* (height, and width) for 1-layer configuration, multiplied height for 2- and 4-layers configurations. The manufacturer's recommended temperature profile has been applied (Figure 5.8).

Another main physics for the multiphysical VBO process modelling is the heat transfer equation (Equation [2.15]) that governs cure kinetics and viscosity of resin system. The results that are calculated based on averaged viscosity and degree of cure in domains, Figure 5.19, shows that models for degree of cure and viscosity, can provide consistent results.



Figure 5.19. Viscosity and degree of cure results for numerical experiments

Due to vacuum bag pressure applied on prepregs, the initial thickness of prepregs are decreased depend on total porosity change. The volumetric strain rate in Equation [2.20] serves to calculate in situ through thickness change of 1, 2 and 4 layers of prepregs. The percentage of thickness change for all 3 scenarios shows (Figure 5.20) that influence of temperature profile on thickness change is obvious. The number of prepreg layer is ensured incrementally increasing the percentage of total thickness change during VBO process.



Figure 5.20. Initial thickness change percentages for 1, 2 and 4 Layer

5.3. Parametric Study for the void comparison

The multiphysical VBO process model calculates resin impregnated area due to capability of instantaneous resin flow front tracking in through thickness of 2D prepreg. After implementing multiphysical model on 1,2 and 4 layers of prepreg, set of numerical studies are carried out for temperature profile parameters (Table 5.8) in order to find total resin impregnation area proportion to total prepreg area. The parameters in parametric study have been selected while the other parameters being constant with respect to the reccommended temperature profile Figure 5.8.

Parameters	Values
Initial Cure Temperature	65,75,85,95, 105 °C
Post Cure Temperature	100, 110, 120, 130, 140 °C
Ramp Rate	1, 2, 3, 5, 10 °C/min
Dwell Time	40, 50, 60, 70, 80 min

 Table 5.8. Parameter ranges for numerical experiments

Impregnation in VBO process is highly depends on initial cure temperature because, viscosity of resin reaches minimum level in this temperature range that yields higher resin impregnation [26]. Initial cure temperature should be high enough to provide impregnation, less enough for not fully cured [5]. In

Figure 5.21, impregnation of prepreg with different initial cure temperature does not exhibit directly proportional relation, indeed, there is another parameter that limits void ratio, which is likely due to viscosity characteristic of resin system.

Initial Cure Temperature



Figure 5.21. Void ratio results for initial cure temperature parameters

Post cure temperature parameter usually assures final curing in VBO manufacturing process. Prepreg impregnation completes with initial cure temperature and curing starts, then final fully cured parts achieved with post cure temperature [11]. The total impregnated area with variety post cure temperature is not expected to be changed, nonetheless, it is expected that total curing time is decreased. From Figure 5.22, the impregnated area in through thickness of prepreg, does not change significantly, at least, observable numerical trend is not captured.





Figure 5.22. Void ratio results for post cure temperature parameters

Critical effect of ramp rate during VBO process comes from relation of the viscosity and the degree of cure. Ramp rate determines the time for both impregnation and curing [6]. Low ramp rates slow total manufacturing cycle with lesser void ratio. Figure 5.23 shows that higher impregnation ratio is achievable with lower ramp rates because of time required for both impregnation and curing are more compared to higher ramp rates.



Figure 5.23. Void ratio results for ramp rate parameters

Dwell time is another temperature profile parameter which keeps prepregs in same temperature in a specific time to let resin infused between fibers. The expected result from dwell time parametric studies to obtain ascending trend between 40 min to 80 min for 1, 2 and 4 Layers of OoA prepreg Figure 5.24.



Figure 5.24. Void ratio results for dwell time parameters

5.4. Optimization of Vacuum Bag Only Process

The optimization with the developed multiphysical VBO manufacturing process is detailly explained in Chapter 4. The parameters that the optimization will be conducted on, are also mentioned, given in Table 5.9. In order to standardize the results of optimization study, the parameters are kept same for each study. These parameters are also the recommended temperature profile [44] by the manufacturer KORDSA®. Moreover, the Nelder-Mead algorithm used in optimization studies will be started with these parameters to construct initial simplex, then this algorithm will be decided which action has to be taken.

Parameters	Initial values
Initial cure temperature	85 °C
Post cure temperature	120 °C
Ramp rate	$2 {}^{\circ}\mathrm{C}/dk$
Dwell Time	60 <i>dk</i>

Table 5.9. The initial parameters used for the optimization studies

5.4.1. Optimized Temperature Profile for 1- Layer

The developed model for 1-layer of prepreg system has been solved and the parametric study has obtained. Next, the optimization study with the Nelder-Mead algorithm is applied on the 1-layer model to find optimum temperature profile parameters to minimize void content or maximize resin impregnation during VBO process. The objective function defined for the optimization study is aimed %99 as described the surface area of the resin impregnated area over the solution domain (Equation [5.1] and [5.2]). Optimality tolerance for the algorithm is chosen to be 0.01, means that the result can vary only %1. The defined constrained is to have 0.96 degree of cure in the domain. The initial step size for the initial and post cure temperature 10 °C, dwell time 10 *min*, the ramp rate 0.5 °C/*min* has chosen.

The evolution of these parameters can be seen in Figure 5.25. As can be seen, the ramp rate started from 2 °C/*min* and significantly needed to decrease with almost each iteration, ended up to 1 °C/*min* aroung 25. iterations. The initial cure temperature (med_limit in the graph) is firstly increased then, started to decrease up to 77.446 °C in around 30. iterations. The post cure temperature (up_limit in the graph) started with 120 °C, ended up approximate 130 °C after 30. iterations. The dwell time is converged to 68 *min*. The parameters approximately converged to a constant number after 30. iterations, despite the objective function, the parameters become almost constant. However, the objective function showed different behavior, even though the parameters are became almost constant, the objective function significantly varied (Figure 5.26).



Figure 5.25. Temperature profile parameters evolution in Nelder-Mead algorithm for 1layer prepreg



Figure 5.26. Objective function change during each iteration of Nelder-Mead algorithm for 1 layer prepreg

The optimization study results, the converged numbers for the parameters, can be found in Table 5.10. The initial temperature profile that the Nelder-Mead algorithm simplex constructed, and the obtained parameters in Table 5.10 can be visualized in Figure 5.27. To compare the results, the recommended profile has lesser total time, but the optimized profile needed higher time to complete the process with about 0.92 resin impregnated area as opposed to 0.87 in the recommended profile. The increase in resin impregnated area is about %5 in total.

Parameters	Optimized Values
Initial cure temperature	77.446 °C
Post cure temperature	132.72°C
Ramp rate	1 °C/min
Dwell Time	68.64 min

Table 5.10. Optimized temperature profile parameters for 1 layer prepreg



Figure 5.27. The comparison of the recommended temperature profile and optimized temperature profile achieved by the Nelder-Mead algorithm for 1 layer prepreg

5.4.2. Optimized Temperature Profile for 2- Layer

The same procedure applied in 1-layer multiphysical VBO process modelling developed in this thesis, similarly, is performed on 2-layer model with the same conditions from, boundary conditions to implicate VBO process, to optimization study in order to standardized to results of optimization studies. The result of temperature profile parameters for 2-layer solution has similar trends with minor changes. Indeed, the ramp rate is reduced to about 1 °C/*min*, the dwell time slightly increased for 2-layer solution from 68.64 *min* to 74.64 *min*, the initial cure temperature is increased from 77.446 °C to 85.47 °C, and lastly the post cure temperature is a considerable reduced from 132.72°C to 123.14°C. The change of optimized parameters with each iteration is seen in Figure 5.28, and the last converged values in Table 5.11.



Figure 5.28. Tempreature profile parameters evolotion in Nelder-Mead algorithm for 2 layer prepreg

 Table 5.11. Optimized temperature profile parameters for 2 layer prepreg

Parameters	Optimized values
Initial cure temperature	85.47 °C
Post cure temperature	123.14°C
Ramp rate	1.04 °C/min
Dwell Time	74.64 min

The objective function for 2-layer optimization study is started with 0.9 resin impregnated area with proportional to total computation area, ended up to about 0.93 as can be seen in Figure 5.29. The change of resin impregnated area increases about %3 with the optimization study. The comparison of the recommended profile and the optimized temperature profile is visualized with Figure 5.30.


Figure 5.29. Objective funcion change during each iteration of Nelder-Mead algorithm for 2 layer prepreg



Figure 5.30. The comparison of the recommended temperature profile and optimized temperature profile achieved by the Nelder-Mead algorithm for 2 layer prepreg

As a summation, the optimization study on 1 and 2 layers of multiphysical VBO manufacturing process modelling is performed with the Nelder-Mead algorithm. The numerical working priciple of the algorithm is investigated and then the optimization study is conducted. The temperature profile parameters are aimed to be optimized to maximize the resin impregnation over the prepreg through thickness. The objective function definition, the Nelder-Mead algorithm parameters, are proved to achieve better

impregnation rates as numerically with the optimization studies. However, the aimed objective function was that %96 of the prepreg has to be impregnated with resin. The algorithm could not be able to reach that impregnation rates. Eventhough the optimization study is proven to be working, the detail working on the Nelder-Mead algorithm should be done in order to achieve higher and realistic objective function.

Chapter 6

SUMMARY, CONCLUSION AND FUTURE WORK

6.1. Summary and Conclusion

In this thesis, the multiphysical model for OoA prepregs by integration of resin flow, heat transfer and consolidation are developed to establish new methodology for achieving void reduced parts, specifically for aerospace industry. The main governing physics and empirical relations for describing material behavior of fiber architecture, resin system and process parameters (temperature profile) with proper boundary conditions are applied for 1-, 2- and 4-layers of OoA prepreg, then parametric numerical experiments performed on initial, post cure temperature, ramp rate, and dwell time parameters of temperature profile. The results of numerical experiments are evaluated based on numerical void ratios and compared with literature.

Temperature profile parameters showed sufficient results compared to conventional OoA prepregs that are investigated in literature. Impregnation of VBO process is achieved mostly in initial cure temperature. The second phase of temperature profile, post cure temperature, only used to obtain fully cured parts. The increasing in ramp rate led to decrease void ratio for 1, 2 and 4 layers of prepreg, also arises to incomplete impregnation. The dwell time for successful impregnation with considering cure kinetics and consolidation physics, reveals directly effective parameter during VBO process.

In general, multiphysical modelling of OoA prepregs facilitates adequate numerical results for resin flow, heat transfer and consolidation behavior during VBO process. The

modelling approaches shows that multiphysical modelling method can capture realistic VBO physics output, in addition to reveal time of air evacuation channel progression lead to void initiation.

The following conclusions are obtained in this thesis,

1. The developed model proved that the multiphysical modelling of VBO process applied in 2D computational domain numerically can capture resin flow, cure kinetics and consolidation physics simultaneously.

2. VBO manufacturing process can be achieved for single and multilayered prepreg systems. The developed model is applied on 1-, 2- and 4-layers of OoA prepreg systems.

3. The multiphysical assessments of the models are presented to prove that the literature knowledge on the temperature profile parameters is obtained with the multiphysical VBO process modelling on 1-, 2- and 4-layers on i) permeability to fiber volume fraction, ii) degree of cure and viscosity, iii) the percentage of initial thickness change.

4. From the initial cure temperature results, the impregnation is increased up to a temperature point, but the increasing in the initial cure temperature is inversely affecting after a certain point.

5. The post cure temperature does not respond as much as initial cure temperature on the impregnation, it is usually maintained to increase degree of cure in the parts.

6. The ramp rate is vital process parameter in temperature profile of VBO manufacturing process. Lower ramp rates attain higher processing time in temperature profile so that the impregnation may successfully be completed with much more processing time, inversely, higher ramp rates provides earlier increasing in degree of cure, even though the impregnation is not finished.

7. Dwell time in temperature profile of VBO process shows a directly proportional relation with the impregnation, hence, the increasing in dwell time ensures better impregnation during VBO process.

8. The optimization study with Nelder-Mead algorithm can be used to obtain optimized process parameters on VBO process. The determination of the effective process parameters on VBO process is offered to be i) initial cure temperature, ii) post cure temperature, iii) dwell time, iv) ramp rate. The optimization approach with Nelder-Mead algorithm, can achieve better impregnation ratios, and the composite manufacturing processes can be improved with optimization approaches as long as the model can provides realistic impregnation ratios.

9. Even though, the objective function has been set to reach %96 resin impregnation, the algorithm is achieved approximately maximum of %93 resin impregnation. The reason not to reach target objective function may be caused by the numerical instability of the developed model or the parameter definition error for algorithm by the user.

10. The integration of governing physics in VBO manufacturing process can be implemented to interpret process itself in numerical environment and be useful tool to improve VBO manufacturing process on determination of composite manufacturing process design.

11. Apart from numerical results, multiphysical modelling of VBO process in 2D domains reveals air evacuation channel development, void initiation mechanism that provides locational prediction for voids, therefore, voids are high probably to be occurred in mold sides.

6.2. Future Works

The following titles can be performed to improve the mathematical description of VBO process:

- the acquisition of permeability in prepregs with the gas (air) permeability experiments
- the consideration of the magnitude of pressure distribution over small part of prepregs
- the numerical improvement on consolidation characteristic of prepregs

• the addition of debulking process for multilayered prepreg system can be added to developed multiphysical VBO process model.

Following the current thesis, the implemented numerical scheme can be performed:

- the solution approaches can be performed with other commercially available software, such as ANSYS® FLUENT®, ALTAIR® etc.
- the formulations can be a custom built for the better computational performance with, for example, MATLAB ®

The following investigations can be added into COMSOL Multiphysics®,

- the various numerical equations for permeability, pressure and change of porosity
- the performance of model on the complex geometries can be implemented
- the improvement on the numerical stability and performance
- the effect of variations on the process parameters of VBO can be extended study
- the standardized numerical road map for the flow front tracking can be investigated
- the solution can be furthered in three-dimensional configuration

In order to further the thesis study, the experimental works that should be done in future:

- the validation of numerical void content with experimental Micro-CT void results
- the determination of the initial vacuum pressure, and initial permeability with experiments
- the modification of the predefined parameters to calibrate multiphysical VBO process model with experimental void content results in prepreg

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