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Numerical Modelling and Optimization of Non-isothermal, Rigid Tool Liquid Composite Moulding Processes

By

Abhishek Gupta

Abstract

The term Liquid Composite Moulding (LCM) is used to define a class of composites manufacturing methods in which a liquid resin is injected into a closed mould containing a dry fibrous reinforcement. Resin Transfer Moulding (RTM) and Compression RTM (CRTM) are rigid-tooled subsets of this class which allow the production of high quality composite parts that are finished to tight dimensional tolerances. However, the design of the manufacturing cycle for these rigid-tool processes involves a large number of design variables which must be carefully chosen in order to minimize cycle time, capital layout and running costs, while maximizing final part quality. These objectives are principally governed by two separate phases of the cycle, namely the resin filling and curing phases, which are strongly coupled in the case of entirely non-isothermal production cycles.

The distribution of design variables over largely disparate phases has so far prevented researchers from developing an integrated approach towards complete process optimization. The work presented in this thesis is focussed towards filling this lacuna, and can be divided into two major sections. The first deals with the investigation of accurate Finite Element (FE) models for solving the coupled flow/energy/species equations, which govern the convection-dominated resin flow through the fibrous medium during the filling phase. It is well known that Partial Differential Equations (PDEs) of this kind are difficult to solve using the classical Galerkin FE technique as it leads to spurious oscillations in the field variable. Therefore, a set of advanced stabilized techniques, most of which allow discontinuities either in the FE weighting functions or in the field variable itself, are suitably modified and tested in order to find the one scheme that best suits non-isothermal LCM simulations. In the second part of the thesis a comprehensive framework for optimizing the complete composites manufacturing cycle is developed, one which encompasses both the mould filling and the resin cure phases. Independently optimizing either phase often leads to conditions that significantly restrict or adversely affect the progress of the other. In light of this fact, a novel approach is suggested for optimizing the dual-phase multicriteria problem by modelling it as a static Stackelberg game with two virtual decision makers (DMs) monitoring the filling
and curing phases, respectively. The game is simulated through a Bilevel Multiobjective Genetic Algorithm (BMOGA), in conjunction with an Artificial Neural Network (ANN) based surrogate model as a substitute for the otherwise computationally expensive FE mould filling simulation.
Acknowledgement

As part of Hindu culture, it is considered auspicious to chant the name of Ganesha (the Elephant God) prior to embarking on any important journey. Not being at all religious myself, I begin this thesis by naming two humans who are more than gods to me. I call them Ma and Bapi; my parents.

First and foremost I wish to thank Assoc. Prof. Piaras Kelly. Moving to a foreign land to begin research on an unfamiliar subject initially seemed like a daunting task, but you made me feel at home right from the get go. I greatly appreciate your patience and encouragement, particularly during the many detours that I took. Your guidance has been invaluable in shaping some of those into the contents of this thesis. Also, thanks for the apple crumble recipe and I’m terribly sorry about your bicycle!

To Prof. Matthias Ehrgott, the optimization guru, thank you for converting a complete novice at multicriteria optimization into someone who can now claim to know a little bit.

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Thanks to Dr. Andrew Walbran, whose prior research is the source of all the critical experimental data that I’ve used. Many thanks for making my trip to Munich such a memorable one, particularly by enlightening me with your profound knowledge of fermented cereal grains.

To all my colleagues here in 439 325 - 70 Symonds Street, a big thanks for creating such a wonderful work environment. The past few years of my life have almost exclusively been spent in this room. I’ve managed to keep my sanity through these thanks solely to the long hours of random conversation with Imran over countless coffee breaks. I wish him, and all the others, the best in their future endeavours.
Finally, I acknowledge that among all my accomplishments over the past few years as a grad student, the greatest has been discovering the one person I want to spend the rest of my life with, Aakriti. I apologize for the heartache I've caused through my absence and thank you from the bottom of my heart for your support and patience.
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Last updated: 25 March 2013
Table of Contents

Abstract ............................................................................................................................................. i
Acknowledgement ........................................................................................................................... iii
List of Figures .................................................................................................................................... xv
List of Tables ....................................................................................................................................... xvii
Introduction ........................................................................................................................................ 1
  1.1 Background and Motivation ........................................................................................................ 1
  1.1.1 The RTM cycle ....................................................................................................................... 3
  1.1.2 The CRTM cycle ..................................................................................................................... 4
  1.1.3 Why another simulation package? ......................................................................................... 5
  1.1.4 Shortcomings of existing optimization techniques .............................................................. 8
  1.2 Research Objectives and Thesis Outline ................................................................................... 10
Numerical Modelling of Isothermal Flow ....................................................................................... 15
  2.1 Governing Equations .................................................................................................................. 15
  2.2 Numerical Solution Procedure .................................................................................................. 16
    2.2.1 The Discrete Nonnegativity Principle .................................................................................. 18
    2.2.2 Non-conforming FE technique ............................................................................................ 18
  2.3 Validation Study ......................................................................................................................... 23
    2.3.1 RTM process simulation ....................................................................................................... 24
    2.3.2 CRTM process simulation .................................................................................................... 26
    2.3.3 Discussion on mass conservation ....................................................................................... 27
  2.4 Summary ..................................................................................................................................... 28
Numerical Modelling of Non-isothermal Flow .................................................................................. 29
  3.1 Governing Equations .................................................................................................................. 29
  3.2 General Numerical Approach .................................................................................................... 32
  3.3 Finite Difference Formulations .................................................................................................. 37
    3.3.1 Through-thickness heat conduction by the Crank-Nicolson method ................................. 37
    3.3.2 Runge-Kutta method for updating resin cure states .......................................................... 39
  3.4 Optimal Galerkin FE Based Convection-Diffusion Algorithms ................................................ 40
    3.4.1 Inadequacy of the classical Galerkin FE method ............................................................... 42
    3.4.2 Streamline Upwind Petrov-Galerkin .................................................................................. 46
    3.4.3 Beyond-SUPG ...................................................................................................................... 47
    3.4.4 Mizukami-Hughes Petrov-Galerkin ................................................................................... 48
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.4.5 FE method based Flux-Corrected Transport</td>
<td>53</td>
</tr>
<tr>
<td>3.4.6 Mixed Galerkin /Lesaint-Raviart</td>
<td>55</td>
</tr>
<tr>
<td>3.5 Verification and Comparison of Numerical Schemes</td>
<td>59</td>
</tr>
<tr>
<td>3.5.1 Experimental Case 1 - Rectangular Mould Filling</td>
<td>60</td>
</tr>
<tr>
<td>3.5.2 Experimental Case 2 - Circular Mould Filling</td>
<td>62</td>
</tr>
<tr>
<td>3.5.3 Numerical Simulations</td>
<td>64</td>
</tr>
<tr>
<td>3.5.4 Discussion</td>
<td>70</td>
</tr>
<tr>
<td>3.6 Summary</td>
<td>72</td>
</tr>
<tr>
<td><strong>Simulating the Effect of Temperature Elevation on Clamping Force Requirements</strong></td>
<td>73</td>
</tr>
<tr>
<td>4.1 Fibre Compaction Model</td>
<td>73</td>
</tr>
<tr>
<td>4.1.1 Mixed-elastic model</td>
<td>75</td>
</tr>
<tr>
<td>4.2 Simulation of Non-isothermal Rigid Tool LCM Processes</td>
<td>76</td>
</tr>
<tr>
<td>4.2.1 Planar-part simulation</td>
<td>78</td>
</tr>
<tr>
<td>4.2.2 Non-planar part simulation</td>
<td>83</td>
</tr>
<tr>
<td>4.2.3 Discussion</td>
<td>84</td>
</tr>
<tr>
<td>4.3 Summary</td>
<td>87</td>
</tr>
<tr>
<td><strong>Bilevel Multiobjective Optimization of LCM Processes</strong></td>
<td>89</td>
</tr>
<tr>
<td>5.1 Considered Design Objectives</td>
<td>89</td>
</tr>
<tr>
<td>5.2 Objective Evaluation Procedure</td>
<td>90</td>
</tr>
<tr>
<td>5.3 Multicriteria Optimization</td>
<td>91</td>
</tr>
<tr>
<td>5.4 Bilevel Multiobjective Optimization</td>
<td>92</td>
</tr>
<tr>
<td>5.4.1 Adaptation of the LCM process optimization problem</td>
<td>93</td>
</tr>
<tr>
<td>5.5 The NSGA-II Algorithm</td>
<td>94</td>
</tr>
<tr>
<td>5.5.1 Fast nondominated sorting algorithm</td>
<td>95</td>
</tr>
<tr>
<td>5.5.2 Crowding distance measurement</td>
<td>96</td>
</tr>
<tr>
<td>5.5.3 Binary tournament selection</td>
<td>96</td>
</tr>
<tr>
<td>5.5.4 Crossover operator</td>
<td>96</td>
</tr>
<tr>
<td>5.5.5 Mutation operator</td>
<td>97</td>
</tr>
<tr>
<td>5.5.6 Migrating nondominated solutions to the RI</td>
<td>98</td>
</tr>
<tr>
<td>5.6 The BMOGA</td>
<td>99</td>
</tr>
<tr>
<td>5.7 Summary</td>
<td>100</td>
</tr>
<tr>
<td><strong>Optimization Examples</strong></td>
<td>103</td>
</tr>
<tr>
<td>6.1 Manufacturing a Composite Disc</td>
<td>103</td>
</tr>
<tr>
<td>6.1.1 Determining feasible bounds of the design space</td>
<td>103</td>
</tr>
<tr>
<td>6.1.2 Building a dataset</td>
<td>105</td>
</tr>
</tbody>
</table>
List of Figures

Figure 1.1: Examples of the applications of composite materials............................................. 2
Figure 1.2: Steps involved in the RTM process........................................................................ 3
Figure 1.3: Steps involved in the CRTM process................................................................. 4
Figure 2.1: Non-conforming triangular element................................................................. 18
Figure 2.2: Surface mesh of a quarter of a hemispherical part........................................... 24
Figure 2.3: Comparison of analytical and numerical results for the fluid force evolution during an RTM process........................................................................... 26
Figure 2.4: Numerical solution of fluid force evolution during a CRTM process.................... 27
Figure 2.5: Verification of the mass conservation principle...................................................... 28
Figure 3.1: Through thickness mesh layers and nodes......................................................... 34
Figure 3.2: Linear 1-D asymmetric FE weighting function.................................................. 43
Figure 3.3: Inadequacy of the central differenced FD scheme............................................ 45
Figure 3.4: Partition of an element into vertex and edge zones........................................... 50
Figure 3.5: Flowchart for obtaining perturbations to the weighting functions....................... 51
Figure 3.6: Experimental observations of thermal histories for EXP 1.................................. 61
Figure 3.7: Experimental observations for thermal histories for EXP 2............................... 63
Figure 3.8: Unstructured triangular finite element mesh for EXP 1 and EXP 2..................... 65
Figure 3.9: Numerical simulations using Type 1 algorithms for EXP 1................................. 66
Figure 3.10: Comparison of analytical and Type 1 numerical predictions for EXP 1............. 67
Figure 3.11: Numerical simulations using Type 2 algorithms for EXP 1............................... 67
Figure 3.12: Comparison of analytical and Type 2 numerical predictions for EXP 1............. 68
Figure 3.13: Numerical simulations using Type 1 algorithms for EXP 2............................... 68
Figure 3.14: Comparison of analytical and Type 1 numerical predictions for EXP 2............. 69
Figure 3.15: Numerical simulations using Type 2 algorithms for EXP 2............................... 69
Figure 3.16: Comparison of analytical and Type 2 numerical predictions for EXP 2............. 70
Figure 4.1: Effect of temperature variation on the force evolution and radial fluid pressure distribution for all RTM planar-part simulations......................................................... 78
Figure 4.2: Effect of resin injection pressure and temperature variation on the force evolution curves for planar-part CRTM simulations......................................................... 81
Figure 4.3: Effect of resin injection height and temperature variation on the force evolution curves for planar-part CRTM simulations......................................................... 82
Figure 4.4: Effect of temperature variation on the force evolution curve for all RTM non-planar part simulations............................................................. 83
Figure 4.5: Effect of resin injection pressure and temperature variation on the force evolution curves for non-planar part CRTM simulations........................................ 85
Figure 4.6: Effect of resin injection height and temperature variation on the force evolution curves for non-planar part CRTM simulations.................................................. 86
Figure 5.1: Manufacturing problem summary...................................................................... 90
Figure 5.2: The proposed BMOGA procedure.................................................................... 99
Figure 6.1: A simple Multilayer Perceptron................................................................. 106
Figure 6.2: Summary of the CCA-NN training procedure. ............................................ 108
Figure 6.3: Comparison of CCA-NN predictions against actual function evaluations.... 109
Figure 6.4: Results in objective space of the lower level problem for the composite disc case.......................................................................................................................... 111
Figure 6.5: Force evolution curves for randomly chosen lower level Pareto optimal solutions ........................................................................................................................................ 111
Figure 6.6: Results in objective space of the upper level problem for the composite disc case ........................................................................................................................................ 112
Figure 6.7: Force, temperature and degree of cure evolution curves ......................... 113
Figure 6.8: Finite element mesh of the fireman’s helmet. ............................................. 114
Figure 6.9: Force evolution curves for isothermal filling simulations....................... 115
Figure 6.10: Comparison of CCA-NN predictions against actual function evaluations.. 117
Figure 6.11: Results in objective space of the upper level problem for the fireman’s helmet case ........................................................................................................................................ 118
Figure 6.12: Force, temperature and degree of cure evolution curves for the preferred solution ....................................................................................................................................... 119
Figure A.1: Comparing the effect of increasing Fo on numerical predictions.......... 139
Figure A.2: Comparison of analytical and numerical predictions for through-thickness temperature profiles................................................................. 140
List of Tables

Table 2.1: RTM simulation error analysis .................................................................26
Table 2.2: CRTM simulation error analysis ...............................................................27
Table 3.1: Material properties for EXP 1.................................................................60
Table 3.2: Material properties for EXP 2.................................................................62
Table 3.3: Average runtime comparison of simulations ...........................................71
Table 4.1: Mixed-elastic compaction model parameters .........................................76
Table 4.2: Epoxy resin properties ............................................................................77
Table 4.3: Plan of simulations ..................................................................................77
Table 6.1: Design variable bounds and constraints for the composite disc ............104
Table 6.2: Design variable bounds and constraints for the fireman’s helmet ..........116
Table 6.3: Design variables corresponding to the preferred solution ....................119
Chapter 1

Introduction

1.1 Background and Motivation

A composite is formed when two or more constituent materials, which generally have very different properties, are combined to create a single, often superior, material. Although this definition encompasses a wide variety of naturally occurring as well as artificially engineered materials, the present research is focussed towards synthetic fibre-reinforced polymer (FRP) composites. FRP components provide several advantages over traditional metallic parts; these include high thermal stability and corrosion resistance. However, it is their high strength to weight ratio that is slowly making them indispensable to applications aiming for high energy efficiency, especially in the aerospace and automotive industries (see Figure 1.1).

In order to face the growing demand for FRP composites in an efficient manner, it is important that their manufacturing cycle be optimized so as to minimize costs while maintaining high part quality. To this end, an investigation of rigid-tool Liquid Composite Moulding (LCM) methods, which are popular techniques for high volume production of superior quality FRP components, is carried out in this thesis. A generic LCM process is one in which a liquid thermosetting resin is injected, under pressure, into a closed mould containing a dry fibrous reinforcement. The rigid-tooled subset of these methods comprises the Resin Transfer Moulding (RTM) and Compression RTM (CRTM) processes that are characterised by the use of high stiffness moulds which are assumed to undergo negligible deflection during the entire manufacturing cycle. These methods provide the manufacturer with several advantages when compared to other flexible-tool LCM or open mould techniques; these include high quality surface finish of the part, fulfilment of tight dimensional tolerances and reduced exposure to hazardous solvent emissions. However, the moulds used for these processes are often subject to large internal forces which originate due to the high resin injection pressure and compaction response of the fibrous reinforcement. Therefore, appropriate clamping equipment (e.g. hydraulic
press or perimeter clamps) must be selected (or designed) in order to equilibrate these forces, so as to keep the mould closed and prevent appreciable mould deflection. This prerequisite often demands sophisticated tooling equipment, which subsequently leads to high costs in setting up and running the equipment, thereby placing limits on the applicability of these methods.

Figure 1.1: The BMW i8 concept car (a) and the Boeing 787 Dreamliner (b) are examples of the applications of composite materials in the automotive and aerospace industries.
1.1.1 The RTM cycle

The setup of the RTM process generally consists of a metal mould precisely machined according to the geometry of the part to be manufactured. A preform of the dry fibrous reinforcement is placed into the mould cavity (Figure 1.2a). The mould is closed to the required part thickness thus compacting the preform to the desired fibre volume fraction (Figure 1.2b). The mould, along with the reinforcing fibres, is often heated to a predefined operation temperature after which a thermoset resin, which may also be preheated, is injected into the mould through one or more injection gate(s) (Figure 1.2c). Once the resin reaches the mould-vent(s) filling is discontinued and the resin is allowed to cure (solidify) sufficiently before part extraction (Figure 1.2d).

![Figure 1.2: Steps involved in the RTM process, (a) preform placement, (b) mould closure to required part thickness, (c) resin injection, and (d) resin cure and part extraction [1].]
1.1.2 The CRTM cycle

CRTM is very similar to RTM, but with an additional wet fibre compaction phase incorporated into it [1-7]. A schematic of the CRTM process is depicted in Figure 1.3. Unlike in RTM, the mould is not closed to the final part thickness prior to resin injection. After a measured quantity of resin has been injected, the injection gates are shut and the mould is closed to the desired thickness, thereby forcing the resin
through the remaining dry parts of the preform using compression driven flow. The increased preform porosity during injection, resulting from partial mould closure, allows the resin to flow freely and permits faster cycle times in CRTM as compared to RTM [1, 8]. However, the internal forces exerted on the mould tools during the secondary compression stage of the CRTM process are often much larger than that exerted during an RTM cycle [1, 2, 8]. As a result, there may be a significant price to pay for the reduced cycle time, in the form of a further increase in the cost of tooling equipment required.

1.1.3 Why another simulation package?

To allow manufacturers to reap the benefits of these rigid-tool methods while maintaining affordability, it is important to have accurate means of predicting how different process design variables (such as the thermal conditions of the mould and the resin, resin injection pressure, the mould closure speed during the secondary compression phase of a CRTM cycle, etc.) may affect the efficiency of the production cycle in terms of the time required to manufacture each part and the resources consumed in doing so. With the advent of powerful computational hardware it is now possible to numerically model the underlying physics of these processes to a very high degree of precision and within a reasonable amount of time. Availability of a reliable simulation tool would allow the manufacturer to design optimized production cycles without the need to undergo an experimental trial and error procedure, which often leads to significant overhead in terms of costs and time. All these factors provide strong motivation towards the development of an all-inclusive simulation package for RTM and CRTM processes, one which is capable of modelling the flow of the resin through the reinforcing fibres as well as predicting the evolution of the internal forces experienced by the moulds. Although substantial work has been done in the composites manufacturing research community for the development of Finite Element (FE) based numerical procedures for simulating LCM processes [9-11], it is only more recently that a simulation tool has been developed, at the University of Auckland, that includes the evaluation of forces experienced by the mould tools under isothermal processing conditions [2, 12, 13].

The dearth of such force predicting software is primarily due to the requirement that an accurate prediction of the tooling forces generated can only be achieved
through a compaction model which suitably duplicates the response of the fibrous reinforcement being used in the particular process. Fibrous materials have been characterised to respond in different ways; ranging from a non-linear elastic response [14, 15] to more elaborate models, namely the mixed-elastic model [1, 2, 12, 13] and the compression speed dependent viscoelastic model [2, 16-18]. Among these, the mixed-elastic model is considered computationally efficient [19] and has been shown to make accurate predictions for a wide range of rigid-tool LCM simulations [2, 20]. It is therefore used often within SimLCM, the LCM process simulation package of the University of Auckland [12].

Along with tooling force prediction a complete simulation package must also allow the modelling of non-isothermal processing conditions. Industries facing high production demands generally use preheated mould and resin systems to speed up the manufacturing cycle. This mainly results from the high sensitivity of the resin viscosity to its thermal condition. As the resin flows, it absorbs heat from the fibres and the mould walls. This causes its viscosity to drop significantly, allowing faster fibre wet out, and hence shorter fill times. However, increased temperature also accelerates the exothermic resin polymerization reaction, i.e. the cross-linking of the resin monomer molecules into their polymeric form. An increase in the degree of resin conversion (or degree of cure) is always accompanied by an increase in the resin viscosity. In some cases the viscosity increase due to curing may dominate the drop due to the temperature increase, even causing the resin to gel and stagnate. An erroneous choice of mould temperature may therefore cause the resin to overheat and cure prematurely, leading to a degraded polymer matrix and/or the existence of deleterious macroscopic voids within the manufactured part. A successful process, therefore, depends heavily on the chosen thermal conditions of the resin and the mould.

It is evident that a numerical model that accurately predicts the temperature profile of the resin-fibre system is critical for designing an efficient manufacturing cycle. The flow of the resin through the pre-heated mould and fibre bed is a highly convection-dominated phenomenon. It is well known that Partial Differential Equations (PDEs) governing phenomena of this type are difficult to solve using conventional numerical schemes, e.g., the Central Finite Differencing scheme and its
FE equivalent – the classical Galerkin FE, as these methods lead to spurious oscillations of the field variable [21, 22] (field variables in the case of LCM simulations include the temperature field as well as the degree of cure distribution within the mould during filling). Over the years, several numerical procedures have been proposed by researches to find physically correct solutions to the convection-dominated flow problem [21-37]. Many of these techniques employ the FE method and attempt to stabilize the numerical predictions by allowing asymmetries or discontinuities in the FE weighting functions [21, 22, 33, 34], or discontinuities in the field variable itself [30-32]. Although significant improvement is achieved over the classical Galerkin FE approach, these methods may still lead to small over/under-shoots in the neighbourhood of sharp gradients in the field variables. This happens because the FE coefficient matrices obtained through these methods do not always satisfy monotonicity properties – a set of conditions placed on the coefficient matrix that preclude the existence of any spurious numerical oscillations [38]. In order to further suppress the small oscillations slope limiting strategies (i.e. limiting the gradient of the field variable within an element) have been developed [39, 40], along with the development of advanced nonlinear stabilization techniques which enforce monotonicity conditions on the FE coefficient matrix. However, it can be argued that the slope limiting techniques are based on ad-hoc arguments that may not accurately represent the underlying physics and can often exhibit shortcomings like the violation of global conservation of flux [34]. Moreover, these techniques, along with the nonlinear ones, may become exceedingly time consuming in the case of unsteady flow problems as element-wise slope corrections or nonlinear iterations would have to be performed within each loop of the flow time steps.

Despite the existence of a large body of literature on the physically correct numerical simulations of convection-dominated flow problems, only a handful of the proposed methods have been tested within an LCM setting [42-46]. Even among those tested, there is no one scheme that has been universally accepted as being best suited for non-isothermal LCM simulations. This is essentially because a trade-off must be made between solution accuracy and efficiency, and the weights given to these two simulation objectives may vary from case to case. While some schemes
give physically acceptable solutions at relatively low computational cost, the nonlinear schemes provide high accuracy but with the downside of being computationally intensive. In summary, it can be seen that there exists a need for identifying either a single or at least a small set of preferred numerical schemes which outperform all others in terms of solution accuracy and efficiency when applied to the simulation of a non-isothermal LCM filling phase.

1.1.4 Shortcomings of existing optimization techniques

Having an accurate fill simulation code is only a first step towards complete manufacturing cycle optimization. To guarantee success of the process design the manufacturer must take both the filling and resin cure phases into consideration. The challenge though does not lie in the numerical simulation of the resin cure phase; the equation governing this phase of the process is a parabolic PDE with a source term, the solution to which can be obtained to a high accuracy using a classical Galerkin FE approach [43] or Central Finite Differencing schemes [45]. For the case of entirely non-isothermal processing, the resin filling and cure phases are strongly coupled to one another; the cure and temperature distributions reached within the part at the end of filling form the initial conditions of the cure phase. Therefore, it becomes crucial to devise an optimization strategy which is capable of handling the dual-phase manufacturing cycle in a coupled manner. A majority of the published papers dealing with comprehensive optimization of LCM processes concentrate solely on the curing phase by assuming isothermal filling with minimal resin polymerization [47, 48]; i.e. the resin is assumed to be at room temperature at all points within the mould. Such simplifications may be rendered invalid in more generic situations involving preheated moulds and resin systems, which lead to significant cure and temperature variations throughout the part. Yu and Young [49] used genetic algorithms to propose a coupled approach for obtaining optimal RTM process parameters. However, the dimensions of the design and objective spaces considered in their study are both highly condensed; the resin injection pressure is assumed fixed and only the temperature of the resin and mould walls are considered as design variables, while the minimization of tooling forces is not included in the objectives. For extending the procedure to include the CRTM case, further design variables will have to be introduced during the filling phase which
will generally have little, if any, effect on the progress of the cure phase. Therefore, the coupled optimization approach, proposed in [49], is considered to be unsuitable for the CRTM case. Another common feature of most optimization algorithms suggested in the literature is that they convert the multicriteria optimization problem into a single objective one by using a weighted sum of the normalized objective values [47-49]. Deciding on the weights and effective normalization parameters implies some prior knowledge, on the part of the manufacturer, of the behaviour of the individual objective functions over the design space. A heuristic judgement of such behaviour, even by an experienced manufacturer, may be deemed to be extremely difficult for the production of parts with varying geometries and utilizing different material constituents. Based on these arguments it is concluded that formulating a single objective optimization problem is impractical, especially when the filling and curing phases are coupled together.

The design of the filling phase of the process involves selecting an optimal combination of design variables, such as the position of injection gates and vents [50-52], the resin injection pressure, the initial cavity height during injection and the speed of mould closure if the height happens to be greater than the desired part thickness [53]. Moreover, for a non-isothermal process, the operation temperatures of the mould and the resin are also added to the list [49]. The chosen combination of these variables governs the mould fill time, the magnitude of clamping force required (and consequently the costs involved in setting up and running peripheral equipment, such as a hydraulic press), and the existence of dry areas within the mould due to improper fibre impregnation [54]. On the other hand, the design of the cure phase, which primarily involves determining the mould temperature profile during curing, affects the total time required for the resin to cure satisfactorily and the generation of residual stresses within the part due to large temperature and cure gradients [47, 48, 55]. Although the objectives of both phases seem largely disparate, they are fundamentally linked to each other in the case of fully non-isothermal processing. Optimization of the filling phase, without considering the cure phase, can lead to thermal conditions which adversely affect the progress of the cure phase. For example, a choice of high mould and/or resin temperatures during filling, which could potentially shorten the fill time, may lead
to overheating and thermal degradation of the resin during the cure phase due to the accelerated exothermic polymerization reaction. However, it should be observed that the objectives of the filling phase are completely independent of the design variables of the cure phase. Similarly, a majority of the design variables of the filling phase have little, if any, consequence on the objectives of the cure phase. It is only the thermal conditions of the injected resin and the preheated mould that interlink the two phases. This feature of the problem precludes a centralized optimization approach in which all the design variables and objective functions involved are included in a single stage of optimization.

1.2 Research Objectives and Thesis Outline

This Doctoral research has two fundamental objectives. The first of these is the identification of a preferred set of physically accurate numerical algorithms for solving the convection-dominated PDEs which arise in the case of non-isothermal LCM processing. In order to achieve this, an in-depth analysis of a collection of FE based numerical algorithms that have so far proven satisfactory in modelling the phenomenon within an LCM simulation setting is carried out. These include the mixed Galerkin/Lesaint-Raviart method [31] which has been utilized in [45, 56], the streamline upwind Petrov-Galerkin (SUPG) method [21] which has been employed in [42, 43], and an FE based flux corrected transport algorithm (FEM-FCT) [29] which has only recently been implemented in [44]. In many cases modifications and/or enhancements are introduced to the forms in which the algorithms are currently in use, in order to adapt them better to LCM simulations. Moreover, the applicability of two other numerical schemes, namely Beyond-SUPG (BSUPG) [34] and the Mizukami-Hughes Petrov-Galerkin (MHPG) [33] method, which have so far remained unexplored by the composites manufacturing research community, is also tested. A comparative study of all the algorithms is conducted based on a number of test cases for which experimental results are available in the literature [43, 57, 58], thereby allowing rigorous verification of their accuracy. The selection of the most preferred set of methods, among the ones considered, has been based on two factors, i.e. their precision as well as their efficiency.

The second objective of this work is the construction of a comprehensive
framework for optimizing the complete composites manufacturing cycle, which includes the mould filling and the resin cure phases. The difficulties arising from the interconnected nature of the two phases, despite the weak link between the objectives of one phase and the majority of the design variables of the other, is overcome by designing a decentralized, game-theoretic framework to model the problem. Two virtual decision makers (DMs) are assumed to monitor the critical phases and interact as the players of a static Stackelberg game. The DM controlling the cure phase is assumed to be the leader, while the one controlling the fill phase is assumed to be the follower. The framework is set up such that neither of the DMs can independently optimize their respective phases without considering the preferences of the other. This approach prevents undesirable outcomes, in terms of part quality and/or manufacturing cycle efficiency, which may arise from performing independent phase optimization. In order to simulate the interaction between the two DMs a Bilevel Multiobjective Genetic Algorithm (BMOGA), based on the popular elitist Nondominated Sorting Genetic Algorithm (NSGA-II) [59], is developed. Since a closed form analytical expression for the objective functions is not available a classical optimization procedure cannot be used. Moreover, a genetic algorithm is preferred over other kinds of metaheuristics as its multicriteria version (i.e. NSGA-II) is well established as being an efficient routine for a large class of optimization problems [60].

Multicriteria optimization has certain unique features which make it extremely useful for the problem at hand. Unlike single objective optimization, wherein a single optimal solution is obtained, the multicriteria approach provides the final result in the form of a set of Pareto efficient solutions [61]. A solution is categorised as being Pareto efficient if an improvement in one of its objectives is necessarily accompanied by a worsening of at least one other [62]. Moreover, the Pareto efficient set contains a subset of properly efficient solutions [62]. In [63] it was shown that if the feasible set in objective space is assumed to be convex, a solution is properly efficient if and only if the solution is optimal for a reduced single objective problem with some strictly positive objective weight combination. This implies that, at least in theory, the solution of a multicriteria optimization problem includes every positive objective weight combination of a single objective problem.
As a result, no prior decision is required on the objective weights or the objective normalization parameters, thereby making any \textit{a priori} knowledge of the behaviour of the objective functions unnecessary.

However, it is noted that the NSGA-II algorithm typically requires at least a few thousand function evaluations to find good solutions, those which are close to the Pareto Frontier [59]. It has also been shown in [64] that the number of lower level function evaluations necessary for a genetic algorithm-based solution to a bilevel multiobjective problem may go up to a few million. Consequently, despite the fact that steps have been taken to minimize the computational cost of the FE fill simulation code, it remains too expensive to be used for function evaluations of the lower level problem. This obstacle is overcome by running the FE simulation only at a few hundred points in the design variable space. The points are chosen through an optimized technique which ensures complete, stratified coverage of the design variable space [65]. The data from these points is then used to train an Artificial Neural Network (ANN) [66] which is subsequently employed as a surrogate to the FE simulation. ANN has been used within an RTM setting previously in [67], where the neural network was trained on an experimentally obtained dataset and was integrated with a genetic algorithm for RTM process optimization. The rapid function evaluations performed by the ANN at the lower level makes the BMOGA based game-theoretic approach computationally feasible for LCM process optimization.

In summary, the two major aims of this research are: 1) Identifying a set of numerical schemes that are best suited for implementation in a simulation package that can model non-isothermal rigid-tool LCM processes, with the added capability of making tooling force predictions; and 2) Constructing a decentralized framework that includes the filling and curing phases of a composites manufacturing cycle, for complete process optimization.

This thesis has been divided into two parts, with each part tackling a separate research objective. Part 1 (Numerical Modelling), which deals with the numerical modelling of resin flow, comprises Chapters 2-4. Part 2 (Optimization), which deals with the optimization of the composites manufacturing cycle, is presented over
Chapters 5 and 6. The overview of Part 1 is as follows:

- Chapter 2 introduces the equations governing resin flow during an isothermal, rigid-tool LCM process and describes the FE scheme adopted for their solution.

- Chapter 3 extends the governing equations to the case of non-isothermal filling. The general solution approach is described, followed by descriptions of each algorithm applied to the convection-dominated flow problem. Experimental test cases are introduced for which analytical solutions are derived. The data is then used to rigorously verify the numerical approach in general and compare the different algorithms considered.

- Chapter 4 first introduces a mixed-elastic fibre compaction model which suitably mimics the behaviour of the fibrous reinforcements being considered in this research. The model is then used together with the FE fill simulation code to study the effect of temperature elevation on clamping force requirements during rigid-tool LCM processes for a planar and a non-planar part.

The outline of Part 2 is described next:

- Chapter 5 contains the mathematical definition of a bilevel multiobjective optimization problem and how the composites manufacturing problem can be made to fit into this framework. Moreover, the chapter provides a detailed description of the NSGA-II based BMOGA used for its solution.

- Chapter 6 applies the BMOGA to a couple of test cases: 1) for manufacturing a simple planar part and 2) a complex industrial part. The chapter also discusses the steps involved in building the surrogate to the fill simulation code.

The thesis is then concluded with principal achievements of the research and suggestions for future work.
Part 1

Chapters 2-4

Numerical Modelling
Chapter 2

Numerical Modelling of Isothermal Flow

In this chapter the governing PDE is derived for the flow of a liquid resin through a fibrous reinforcement during an isothermal rigid-tool LCM process. Different numerical strategies applicable for obtaining an approximate solution to the PDE are discussed, along with the motivation behind the selection of an FE based numerical approach. A detailed mathematical description of a non-conforming FE scheme employed in this work is also presented. The chapter concludes with a validation study carried out for the manufacture of a hemispherical part, for which analytical solutions are derived in order to provide a basis for comparison.

2.1 Governing Equations

The mass conservation/continuity equation for a thickness-varying LCM process can be expressed as follows \[\nabla \cdot (hu) = -\frac{\partial h}{\partial t}.\] (2.1)

Here \(h\) represents the local thickness of the mould cavity in which the reinforcing fibres are placed, and \(u\) is the volume averaged (or Darcy) velocity. The velocity \((u)\) can be obtained from the fluid pressure profile by applying Darcy's law \[\frac{K}{\mu} \nabla p ,\] (2.2)

where \(K\) is the in-plane permeability tensor, \(p\) represents the resin pressure profile and \(\mu\) is the resin viscosity. For an isothermal process the resin viscosity does not vary spatially or change over time. Note that Darcy's Law is valid only for the case of Stokes flow for which the Reynolds number \((Re)\) is low, i.e. \(Re < 1\). Fortunately, the resin flow occurring in LCM processes falls into this category; which makes Darcy's law suitable for modelling the phenomenon. An important consequence of the low \(Re\) is that the flow is clearly laminar. This point shall be utilized in Chapter 3 while introducing the numerical scheme for tackling non-isothermal processing.
Substituting Eq. (2.2) into Eq. (2.1) gives the final elliptic PDE governing the resin flow:

\[ \nabla \cdot \left( h \frac{K}{\mu} \nabla p \right) = \frac{\partial h}{\partial t}. \]  

(2.3)

Notice that in Eq. (2.3) fluid flow in the through-thickness direction is essentially ignored. This is the standard assumption made in the manufacture of relatively thin composite parts [68] in which the in-plane permeability of the fibrous reinforcement does not vary through the part thickness. Moreover, for the assumption to hold for CRTM, no air gap should exist between the mould wall and the preform during resin injection.

Also observe that for the complete RTM cycle and the injection phase of the CRTM cycle the right hand side of Eq. (2.3) is zero as the mould wall remains stationary, thereby keeping the cavity thickness constant. It is only during the final mould closure phase of CRTM that temporal thickness variations are involved.

2.2 Numerical Solution Procedure

FRP components can have significant geometric complexity. Unstructured meshes permit such complex geometries to be modelled with relative ease. Therefore, a numerical solution procedure is sought that can be applied over unstructured meshes. This requirement immediately precludes the selection of the Finite Difference (FD) method as it requires a structured rectangular grid. The Finite Volume (FV) scheme is one which can be formulated to allow for unstructured approximations of the field variable. The fact that the field variable is assumed uniform over the interior of every element may lead to an inaccurate computation of gradient information; such information is essential in the case of LCM simulations while tracking the progress of the resin free surface (or flow front) as it flows through the mould. The FE procedure, on the other hand, can be formulated in a way that allows the field variable to vary at least linearly within each element. This allows a straightforward computation of its gradient, which can then be used to efficiently track the progress of the resin front. The Boundary Element Method
(BEM) is another technique which has been employed in conjunction with the Level Set Method (LSM) for the simulation of the RTM process [69]. The BEM requires the construction of a mesh only over the boundary of the flow domain. The reduced dimensionality of the problem therefore makes this method more efficient than the FE scheme for most cases. Additionally, the LSM allows the moving flow boundary to be tracked with very high accuracy, which leads to an accurate representation of the shape of the flow front. This cannot be achieved by the FE approach as it only transfers resin mass from one element to the other without explicitly tracking the front [69]. However, the BEM can only be directly implemented in the case of isothermal filling of a planar mould containing an isotropic reinforcing material [69]. This is because in such situations Eq. (2.3) simplifies to a Laplace equation (taking \( \partial h / \partial t = 0 \), as is the case for RTM) for which the Green’s function is known; this allows the setting up of the discretized form of the surface integral equation prescribed by the BEM. Therefore, for the general case of non-isothermal RTM or CRTM process simulations of non-planar part geometries, the FE technique remains the most preferred approach [9-12]. It is thereby adopted as the fundamental numerical scheme in this research.

It is important to note that since the through-thickness resin flow within the mould is ignored, the problem reduces to a 2-D surface flow. Even for the case of a complex 3-D part, the resin flow remains locally 2-D. Keeping this in mind, the FE formulations throughout the thesis shall be discussed in 2-D Cartesian coordinates only, since a planar element tilted in 3-D space can easily be mapped to a local xy-plane.

In order to solve Eq. (2.3) a triangular mesh with linear basis functions is used for the spatial discretization of the mould cavity. At the free surface of the resin a zero pressure (or atmospheric pressure) boundary condition necessarily exists whereas at an injection port Dirichlet (prescribed resin injection pressure) or Neumann (prescribed resin flux) boundary conditions are applied as per the requirements of the actual physical process. Once the pressure distribution over the flow domain has been obtained by solving the discretized form of Eq. (2.3), Darcy’s law is used to compute the resin velocity within each element. The resin velocities evaluated for the front elements are then used to update the flow front over the
flow time step. The size of the time step of a particular iteration should be sufficiently small to justify a quasi-steady velocity approximation. A viable approach is to set the step size to be equal to the minimum time span necessary for the flow front to advance over at least one element in that iteration. This procedure is repeated until all the elements of the cavity discretization are filled with resin.

2.2.1 The Discrete Nonnegativity Principle

It is observed that the resin pressure must be non-negative throughout the fluid domain. In order to guarantee that the solution of the discrete set of equations obtained through piecewise linear finite elements satisfies this non-negativity requirement, the triangulation must be of the weakly acute type [33], i.e. all interior angles should be less than or equal to π/2. Even though the mesh of a complex geometry may often include obtuse triangles, certain techniques developed in the subsequent section are based on the assumption that all triangles indeed are at least weakly acute.

Figure 2.1: Non-conforming triangular element with Lagrange linear basis functions (e.g. \(N_1\) corresponding to node 1).

2.2.2 Non-conforming FE technique

In this study the non-conforming FE approach [10, 11, 45] is preferred over the
popular conforming FE/Control Volume (FE/CV) method [9, 44, 70]. In the former, non-conforming elements, i.e. the nodes are located mid-side (see Figure 2.1), are used, and only a single grid of elements is needed for obtaining the pressure distribution and progressing the flow front. On the other hand, the traditional description of the FE/CV method employs a pair of grids, one for finding the pressure profile and the other to progress the front, thereby making the method more cumbersome.

Non-conforming elements do not impose \( C_0 \) continuity requirements along the element edges (except at the nodes). As a result the predicted pressure distribution is not continuous along the element edges, a shortcoming that the FE/CV method precludes. Yet, only a single grid is necessary as these elements possess unique local conservation properties. This feature of the non-conforming element shall be shown while describing its mathematical formulation; see Eqs. (2.17-2.22) below.

The approximation of the resin pressure distribution is obtained by applying the weak formulation given in Eq. (2.4), over an element \( \Omega_e \). This procedure is repeated for every element in the flow domain to obtain a set of linear equations, which when assembled represent the completely discretized form of Eq. (2.3).

\[
\int_{\Omega_e} \nabla \cdot \left( h \frac{k}{\mu} \nabla p \right) \, d\Omega_e = \int_{\Omega_e} \frac{\partial h}{\partial t} \, d\Omega_e. \tag{2.4}
\]

Here \( N \) is the Galerkin-type weighting function, i.e. the linear basis functions are themselves used as weighting functions. Its expression corresponding to node ‘i’ is given by,

\[
N_i = \frac{2}{\Delta} \left( A_i + B_i x + C_i y \right), \quad \text{for } 1 \leq i \leq 3. \tag{2.5}
\]

where \( \Delta \) is the area of the triangular element and assuming the coordinates of the \( \ell^{th} \) mid-side node to be given by \((x_i^*, y_i^*)\), the coefficients \( A_i, B_i \) and \( C_i \) are defined as,

\[
A_1 = x_2^*y_3^* - x_3^*y_2^*, \quad B_1 = y_2^* - y_3^*, \quad C_1 = x_3^* - x_2^*
\]
\[
A_2 = x_3^*y_1^* - x_1^*y_3^*, \quad B_2 = y_3^* - y_1^*, \quad C_2 = x_1^* - x_3^*
\]
\[
A_3 = x_1^*y_2^* - x_2^*y_1^*, \quad B_3 = y_1^* - y_2^*, \quad C_3 = x_2^* - x_1^* \tag{2.6}
\]
The resin pressure distribution within an element is given by,

\[ p = \begin{bmatrix} N_1 & N_2 & N_3 \end{bmatrix} \cdot \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}, \quad (2.7) \]

where \( p_1, p_2 \) and \( p_3 \) are the unknown pressures at the three nodes of the element. Since,

\[ \nabla N_i = \begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_1}{\partial y} \\ \frac{\partial N_2}{\partial x} & \frac{\partial N_2}{\partial y} \\ \frac{\partial N_3}{\partial x} & \frac{\partial N_3}{\partial y} \end{bmatrix}, \quad (2.8) \]

the pressure gradient within the element is,

\[ \nabla p = \begin{bmatrix} \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial x} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_2}{\partial y} & \frac{\partial N_3}{\partial y} \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \\ p_3 \end{bmatrix}. \quad (2.9) \]

From Eq. (2.9) and the definition of \( N_i \) it is clear that the pressure gradient remains uniform within the element. According to Darcy’s law this also implies a unique resin velocity (\( u \)) inside the element.

Prior to further reduction of Eq. (2.4) it must be stated that \( h, K, \mu \) and \( \partial h/\partial t \) are all assumed to be uniform over the extent of each element, but may vary from one element to the other.

Integrating Eq. (2.4) by parts and applying the divergence theorem one has,

\[ \int_{\Omega_e} \nabla N \cdot \left( -h \frac{K}{\mu} \nabla p \right) \, d\Omega_e = \int_{\partial\Omega_e} \left( -h \frac{K}{\mu} \nabla p \right) \cdot \mathbf{v} \, dl + \int_{\Omega_e} N \frac{\partial h}{\partial t} \, d\Omega_e. \quad (2.10) \]

Here \( \partial\Omega_e \) is the element boundary and \( \mathbf{v} \) is an outward unit normal to \( \partial\Omega_e \).

Substituting Eq. (2.2) into the right hand side of Eq. (2.10) one gets,

\[ \int_{\Omega_e} \nabla N \cdot \left( -h \frac{K}{\mu} \nabla p \right) \, d\Omega_e = \int_{\partial\Omega_e} \mathbf{u} \cdot \mathbf{v} \, h \, dl + \int_{\Omega_e} N \frac{\partial h}{\partial t} \, d\Omega_e. \quad (2.11) \]

As,

\[ \int_{\Omega_e} N \, d\Omega_e = \frac{\Lambda}{3}, \quad (2.12) \]
Eq. (2.11) takes the following form,

\[ \int_{\Omega_e} \nabla N \cdot \left( -h \frac{K}{\mu} \nabla p \right) \, d\Omega_e = \int_{\partial \Omega_e} N \mathbf{u} \cdot \mathbf{v} \, h \, dl + \frac{\partial h}{\partial t} \Delta. \quad (2.13) \]

The first term on the right hand side of Eq. (2.13) is a boundary flux which represents a *natural boundary condition*.

The element boundary \( \partial \Omega_e \) can be split as,

\[ \partial \Omega_e = \bigcup_{i=1}^{3} \partial \Omega_{ei}, \quad (2.14) \]

where \( \partial \Omega_{ei} \) is the side of the triangular element on which the \( i^{th} \) node lies. Accordingly, from the descriptions of the basis functions provided in Eq. (2.6) it can be seen that,

\[ \int_{\partial \Omega_{ei}} N_i \, dl = \begin{cases} 0, & \text{for } i \neq j, \\ |\partial \Omega_{ei}|, & \text{for } i = j. \end{cases} \quad (2.15) \]

Therefore, while formulating Eq. (2.13) for the \( i^{th} \) node, the natural boundary condition may be reduced as,

\[ \int_{\partial \Omega_e} N_i \mathbf{u} \cdot \mathbf{v} \, h \, dl = \sum_{j=1}^{3} \int_{\partial \Omega_{ej}} N_i \mathbf{u} \cdot \mathbf{v}_j \, h \, dl = \mathbf{u} \cdot \mathbf{v}_i \, h |\partial \Omega_{ei}| = Q_i^+. \quad (2.16) \]

Here \( Q_i^+ \) is the resin flux through \( \partial \Omega_{ei} \). As a result, Eq. (2.13) takes the following form for the \( i^{th} \) node,

\[ \int_{\Omega_e} \nabla N_i \cdot \left( -h \frac{K}{\mu} \nabla p \right) \, d\Omega_e = Q_i^+ + \frac{\partial h}{\partial t} \Delta. \quad (2.17) \]

As all the terms occurring inside the integral sign are assumed uniform within \( \Omega_e \), Eq. (2.17) becomes,

\[ \nabla N_i \cdot \left( -h \frac{K}{\mu} \nabla p \right) \Delta = Q_i^+ + \frac{\partial h}{\partial t} \Delta. \quad (2.18) \]

Substituting Eqs. (2.8) and (2.9) into Eq. (2.18) provides the discretized equation corresponding to the \( i^{th} \) node;
Note that every node, except the ones on the boundaries of the fluid domain, is connected to two triangular elements. Therefore, for each node two equivalent forms of Eq. (2.19) occur, one for each element. Both these expressions are summed to obtain the complete discretized equation for any interior node. During the summation process it is considered that the boundary fluxes must cancel each other out. It is here that the form of the natural boundary condition occurring for the non-conforming FE case ensures that the amount of resin lost by one element is necessarily gained by its adjacent one. In other words, mass conservation properties are strongly imposed locally on the obtained solution.

While assembling the global system of equations it is considered that only those elements which are completely filled with resin form part of the fluid domain. Among these, the ones adjacent to (i.e. sharing a common edge with) partially filled or unfilled elements are considered to be front elements. Moreover, the nodes shared by the filled elements and the partially/un-filled elements are designated the front nodes at which the zero gauge pressure (or prescribed partial vacuum pressure) boundary condition is applied. The system of equations is then solved for the unknown resin pressure values at the element nodes. The nodal pressures are used to compute the resin velocity within each element by applying Darcy’s law. For computing the flow time step, the resin discharge from side $\partial \Omega_{e_i}$ of a front element is obtained by rearranging Eq. (2.18) in the following manner,

$$\left( Q^+ \right)_{\text{front}} = \nabla N_i \cdot \left( -h \frac{K}{\mu} \nabla p \right) \Delta - \frac{\partial h \Delta}{\partial t}.$$  \hspace{1cm} (2.20)

Since,

$$\Delta(\nabla N_i) = \int_{\partial \Omega_{e_i}} \mathbf{v} \, dl,$$  \hspace{1cm} (2.21)

substituting Eq. (2.21) into Eq. (2.20), the resin discharge takes the following form,
Note, since the pressure gradients for the front elements are known, the first term on the right hand side of Eq. (2.22) follows immediately from Darcy’s law. The second term ensures mass conservation when the flow field is divergent, i.e. during the secondary compression phase of the CRTM process.

The discharge from the front elements, as computed via Eq. (2.22), flows into elements which have so far not been completely saturated by the resin. As has been mentioned earlier, the size of the flow time step is determined by the minimum time span necessary for at least one element located adjacent to the front to get completely saturated. Subsequently, using the flow time step and \((Q_i^t)_{\text{front}}\), the fill-factors of the partially/un-filled adjacent-to-front elements are updated. The fill-factor is defined as the ratio of the resin volume contained within the element, to its void volume. For a completely filled element the fill-factor is therefore equal to 1.

It is stated that the obtained expression for resin discharge from front elements is conservative under the assumption that the triangulation is of the weakly acute type. The existence of an obtuse triangle at the front causes negative boundary flux, which violates the physics of the problem. Therefore, in order to maintain the robustness of the simulation algorithm, when a negative boundary flux occurs it is reassigned to be zero. The error induced by this adjustment has been found to be insignificant while using meshes that also include obtuse triangles.

### 2.3 Validation Study

In this section a validation of the non-conforming FE based isothermal resin flow simulation algorithm is carried out for a hemispherical part. The simplicity of the geometry allows the derivation of analytical solutions for this problem, for the case of RTM as well as CRTM. The radius \(R\) of the hemisphere is 0.1 m, and the part has a constant thickness of \(h = 4.7\) mm. The reinforcing material is a glass-fibre continuous filament mat (CFM) which has a fibre volume fraction \(V_f\) of approximately 0.37 at the given thickness. The isotropic permeability of the material is given by the following Carman-Kozeny model,
Here $C$ and $n$ are material parameters which must be determined experimentally. For the CFM used in this study, $C = 1.53 \times 10^{10}$ m$^{-2}$ and $n = 2.63$ [12]. The resin, of viscosity 0.198 Pa.s, is injected from the apex of the hemisphere; through an injection gate which has a radius of 3 mm. Due to the symmetry of the part only a quarter of the hemisphere has been modelled, as shown in Figure 2.2.

Figure 2.2: Surface triangulation of a quarter of a hemispherical part of radius 0.1 m.

### 2.3.1 RTM process simulation

For simulating the RTM cycle it is considered that the resin is injected at a constant pressure of 400.0 kPa (i.e. a Dirichlet boundary condition is imposed at the injection gate). The governing differential equations for this problem are written in a spherical coordinate system:

Darcy’s law can be stated as,

$$
\mathbf{u} = -\frac{K}{\mu R} \frac{d \rho}{d \theta'},
$$

(2.24)

where $\theta$ is the polar angle, measured at the centre of the hemisphere and from the
vertical. Imposing mass conservation/continuity requirements on the resin velocity
the following differential equation is obtained which governs the resin pressure
distribution within the part;

\[
\frac{d}{d\theta} \left( \sin \theta \frac{dp}{d\theta} \right) = 0. \tag{2.25}
\]

The analytical solution of Eq. (2.25) is given by,

\[
p(\theta) = p_{inj} \frac{\log \left( \frac{\csc \theta + \cot \theta}{\csc \theta_{inj} + \cot \theta_{inj}} \right)}{\log \left( \frac{\csc \theta_{front} + \cot \theta_{front}}{\csc \theta_{inj} + \cot \theta_{inj}} \right)}. \tag{2.26}
\]

Here \(p_{inj}\) is the resin injection pressure, \(\theta_{inj}\) is the polar angle of the injection gate
and \(\theta_{front}\) is the polar angle of the resin front. On obtaining the velocity of the resin
front by applying Darcy’s law to the pressure distribution, the relation between the
polar position of the front and the injection time can be derived;

\[
t(\theta_{front}) = \frac{\mu R^2 (1 - V_f)}{K p_{inj}} \left( \cos \theta_{front} \log \left( \frac{\csc \theta_{front} + \cot \theta_{front}}{\csc \theta_{inj} + \cot \theta_{inj}} \right) + \log \left( \frac{\sin \theta_{front}}{\sin \theta_{inj}} \right) \right). \tag{2.27}
\]

From Eq. (2.26) the fluid force \(F_{fluid}\) acting on the upper mould can be computed
according to Eq. (2.28). This is the force that must be exerted vertically by the
tooling equipment to equilibrate the force originating due to the resin injection
pressure (note that the total tooling force also contains a fibre response component
which is not considered here).

\[
F_{fluid}(\theta_{front}) = \pi (R + h)^2 \int_{\theta_{inj}}^{\theta_{front}} p(\theta) \sin 2\theta \, d\theta. \tag{2.28}
\]

Eqs. (2.27) and (2.28) together give the evolution of fluid force with time.

Figure 2.3 shows a FE mesh refinement study, and also compares the analytical
and numerical solutions. On increasing the number of elements the numerical
solution can be seen to converge towards the analytical one. This fact is further
exemplified through an error analysis provided in Table 2.1. In summary, the
agreement between the simulated and analytically obtained curves provides strong
verification of the accuracy of the simulation algorithm while modelling RTM processes.

Figure 2.3: Comparison of analytical and numerical results for the fluid force evolution during an RTM process.

<table>
<thead>
<tr>
<th>Table 2.1: RTM simulation error analysis</th>
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<tr>
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<tr>
<td><strong>Pea</strong>k force (N)</td>
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</tr>
<tr>
<td>Analytical</td>
</tr>
<tr>
<td>Coarse (352 elements)</td>
</tr>
<tr>
<td>Medium (988 elements)</td>
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<tr>
<td>Fine (2360 elements)</td>
</tr>
</tbody>
</table>

2.3.2 CRTM process simulation

While simulating the CRTM cycle it is considered that the resin is injected at a constant injection rate of 6.2e-6 m$^3$/s (i.e. Neumann boundary conditions are imposed at the injection gate throughout the process, with resin flux at the injection gates being zero during the secondary compression phase). The initial cavity height during resin injection is 8.7 mm. During the secondary compression phase the upper mould is closed at 8 mm/min, until the cavity height reaches 4.7 mm. From these values the total mould fill time equates to 30 seconds (injection) + 30 seconds (compression) = 60 seconds. Moreover, an analytical expression can be obtained for the peak fluid force exerted on the mould during the secondary compression phase. It is straightforward to see that this peak force will be reached at the very end of the secondary compression phase, at the instant when the final cavity height is reached. The resin pressure distribution at that instant can be obtained by solving the following differential equation,
\[
\left(\frac{2hK}{\mu h R^2}\right) \frac{d}{d\theta} \left(\sin \theta \frac{d\varphi}{d\theta}\right) = \sin 2\theta. \quad (2.29)
\]

This leads to the pressure distribution being given by,
\[
p(\theta) = \left(\frac{2hK}{\mu h R^2}\right)^{-1} \left(0.5(1 - \cos 2\varphi_{\text{inj}})\log(\cosec \theta + \cot \theta) - \cos \theta\right). \quad (2.30)
\]

The force acting on the upper mould can then be computed according to Eq. (2.28) by replacing \(\theta_{\text{front}}\) by \(\pi/2\). With the numeric values prescribed, the peak force for the present case equates to 3851 N. Figure 2.4 depicts a mesh refinement study for the CRTM case. Moreover, a prediction error analysis is also provided in Table 2.2. Here again, the solution convergence and the close agreement between the numerical and analytical solutions shows that the simulation algorithm is suitably accurate for CRTM simulations as well.

![Figure 2.4: Numerical solution of fluid force evolution during a CRTM process.](image)

<table>
<thead>
<tr>
<th>Table 2.2: CRTM simulation error analysis</th>
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</thead>
<tbody>
<tr>
<td><strong>Peak force (N)</strong></td>
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</table>

**2.3.3 Discussion on mass conservation**

For an LCM simulation software to be of any use it must satisfy the principle of mass conservation, i.e. the numerical algorithm must preclude the spurious creation
or loss of resin mass (or volume). In Figure 2.5 two pairs of curves comparing the total volume of resin injected through the gates up to a given instant in time, to that contained within the mould at that instant, are depicted. The injected volume is computed from the inlet discharge, by applying Darcy’s law on the pressure distribution near the injection nodes, while the contained volume is computed from the instantaneous element fill-factors. Clearly, the curves match almost exactly, thereby verifying that the algorithm indeed satisfies the conservation law. The slight variation occurs only because the simulation code assumes an element to be filled the instant its fill-factor exceeds 0.98.

![Graph showing resin volume over filling time with variations](image)

Figure 2.5: Verification of the mass conservation principle.

2.4 Summary

The governing PDE for resin flow during a generic rigid-tool LCM process has been derived in this chapter. The derivation is based on Darcy’s Law which is combined with the continuity equation. Isothermal processing conditions were assumed throughout. A variety of possible numerical schemes for tackling the problem were discussed and the choice of the FE approach was explained. A complete mathematical description of the non-conforming FE method was presented. This method has been preferred in this research over the traditional FE/CV technique due to its mass conservation properties. Finally, a validation study was conducted to verify the accuracy of the simulation algorithm. Comparisons were made with analytically derived solutions and the performance was shown to be very good.
Chapter 3

Numerical Modelling of Non-isothermal Flow

This chapter presents an extension of the equations governing the fluid flow, discussed in the previous chapter, to the case of non-isothermal LCM processes. This primarily includes the convection-dominated energy and species transport equations. The general numerical procedure adopted for the solution of these equations is discussed. A mathematical description of the classical Galerkin FE method when applied to convection-diffusion problems is presented in order to show the inadequacy of the technique in such situations. This is followed by descriptions of various stabilized Galerkin FE methodologies for accurately modelling the unsteady convection-diffusion phenomenon. In many cases modifications/enhancements are introduced to the traditional structure of the algorithms in order to efficiently handle the non-isothermal LCM processing conditions, while maintaining precision. A set of experimental test cases are introduced and analytical solutions are derived for them under certain simplifying assumptions. The experimental and analytical data is then used to rigorously verify the validity of the general solution approach, along with the accuracy and efficiency of the convection-diffusion algorithms. A key objective of this chapter is to find the most preferred convection-diffusion algorithm, one which provides good accuracy at minimum computational cost.

3.1 Governing Equations

For non-isothermal processes the resin viscosity is no longer spatially uniform. It depends on the local temperature, \( T(x,y,z) \), and degree of cure, \( \alpha(x,y,z) \in [0,1] \). Hence,

\[
\mu \equiv \mu(T(x,y,z) , \alpha(x,y,z)). \tag{3.1}
\]

The following is a widely accepted rheological model that captures this response for simple polymer blends [71, 72],

\[
\mu = A_\mu e^{\epsilon/RT_{abs}} \left( \frac{\alpha_g}{\alpha_g - \alpha} \right)^{a+b\alpha}. \tag{3.2}
\]
Here $R$ is the universal gas constant, $T_{abs}$ is the absolute resin temperature and $\alpha$ is the instantaneous resin conversion. $E_\mu$ (activation energy), $\alpha_g$ (the degree of resin conversion at which it begins to gel), $A_\mu$, $a$ and $b$ are experimentally determined constants. Given that all these constants are positive and that viscosity computations are only necessary while $\alpha < \alpha_g$, it can be seen that in this interval,

$$\frac{\partial \mu}{\partial T_{abs}} < 0 \quad \text{and} \quad \frac{\partial \mu}{\partial \alpha} > 0.$$ \hspace{1cm} (3.3)

Therefore, the viscosity drops with a rise in temperature and increases with a rise in the degree of resin conversion.

As a result of the non-uniformity in the resin viscosity, the PDE governing the resin flow, given by Eq. (2.3) in Chapter 2, takes the following form for a non-isothermal process,

$$\nabla \cdot \left( h \frac{K}{\mu_a} \nabla p \right) = \frac{\partial h}{\partial t}. \hspace{1cm} (3.4)$$

Here $\mu_a$ is the thickness averaged viscosity which at any point $(x_p, y_p)$ is given by,

$$\mu_a = \frac{\int_h \mu(x_p, y_p, z)dz}{h}. \hspace{1cm} (3.5)$$

The 2-D surface flow condition continues to hold for the case of non-isothermal processes under the added assumption that the temperature and degree of cure profiles are symmetric about the part mid-surface. This would be true if the top and bottom mould walls are heated to the same temperature, which is generally the case in practice.

The spatial temperature variation is obtained by solving the following lumped energy equation which assumes the resin and fibre phases to have the same local temperature [45],

$$\rho \ C_p \ \frac{\partial T}{\partial t} + \rho_r \ C_{pr} \ \mathbf{u} \cdot \nabla T + \mathbf{u} \cdot \nabla p = \nabla \cdot \{(\mathbf{k}_e) + \mathbf{k}_d \nabla T\} + \varphi \ \dot{H}. \hspace{1cm} (3.6)$$

The material properties $\rho$, $C_p$, $k_e$ and $k_d$ represent, respectively, the average density,
specific heat capacity, effective thermal conductivity tensor of the resin-fibre system and the thermal dispersion tensor. $T$ is the local temperature and $\phi$ is the local reinforcement porosity. $\dot{H}$ is a source term representing the heat generated during the exothermic resin polymerization reaction.

During numerical simulations, the heat generated due to fluid friction, i.e. $u \nabla p$, is generally neglected [68]. Therefore, the final form of the energy equation is as follows,

$$\rho \ C_p \ \frac{\partial T}{\partial t} + \rho_r C_{pr} \ u \cdot \nabla T = \nabla \cdot \{(k_e + k_d)\nabla T\} + \phi \ \dot{H}. \quad (3.7)$$

The volume averaged material properties for the resin-fibre system are computed as,

$$\rho \ C_p = \phi \rho_r C_{pr} + (1 - \phi) \rho_f C_{pf}. \quad (3.8)$$

$$k_e = k_e I, \quad \text{where} \quad k_e = \left(\frac{\phi}{k_r} + \frac{(1-\phi)}{k_f}\right)^{-1}. \quad (3.9)$$

Here $I$ is the identity matrix and the subscripts $r$ and $f$ stand for resin and fibres, respectively.

The heat transfer phenomenon represented by Eq. (3.7) is convective-diffusive but is dominated by the first order derivative term during LCM processing. This makes it practically unsolvable using the classical Galerkin FE method, as shall be shown in a later section of this chapter.

Unlike Eq. (3.7), the PDE governing the transport of chemical species is purely convective, but with an added source term. However, it poses the same challenges when it comes to finding a numerical solution procedure. The equation is expressed as,

$$\phi \ \frac{\partial \alpha}{\partial t} + u \cdot \nabla \alpha = \phi \ R_\alpha. \quad (3.10)$$

Here $\alpha$ represents the local degree of resin conversion and $R_\alpha$ is the rate of resin
polymerization. This rate is again a function of the local temperature and degree of resin conversion. In order to accurately capture the relationship, Kamal and Sourour [73] proposed the following general model which is widely used to describe the polymerization reaction,

\[ R_\alpha = \frac{d\alpha}{dt} = (k_1 + k_2\alpha^{m_1}) \cdot (1 - \alpha)^{m_2}. \]  

(3.11)

The rate constants \( k_1 \) and \( k_2 \) are expressed in the Arrhenius form as,

\[ k_1 = A_1 \cdot e^{(-E_1/R T_{abs})} \quad \text{and} \quad k_2 = A_2 \cdot e^{(-E_2/R T_{abs})}. \]  

(3.12)

In Eqs. (3.11) and (3.12) \( m_1 \) and \( m_2 \) are catalytic constants, \( E_1 \) and \( E_2 \) are activation energies, \( A_1 \) and \( A_2 \) are constants. On combining these two equations \( R_\alpha \) takes the form,

\[ R_\alpha = (A_1 \cdot e^{(-E_1/R T_{abs})} + A_2 \cdot e^{(-E_2/R T_{abs})} \cdot \alpha^{m_1}) \cdot (1 - \alpha)^{m_2}. \]  

(3.13)

In Eq. (3.13) considering all the constants to be positive and then differentiating it is straightforward to show that,

\[ \frac{\partial R_\alpha}{\partial T_{abs}} > 0. \]  

(3.14)

Therefore, an increase in local temperature accelerates the resin polymerization reaction. This fact, along with the inference drawn from Eq. (3.3), makes it critical to choose an operation temperature which allows fast mould filling without causing the resin to gel prematurely.

It is noted that the rheology and cure kinetics of thermosetting resins can be modelled in a variety of ways. Any chosen model can however be accommodated into the numerical approach in a straightforward manner, as shall be clear through discussions in Sections 3.2 and 3.3.

3.2 General Numerical Approach

The solution of Eq. (3.4) follows the same procedure as described in Chapter 2 (Section 2.2.1). Although for a non-isothermal process the resin viscosity is not
spatially uniform, it is assumed to be more-or-less uniform within each element. The value of the element viscosity is thus computed simply by averaging the thickness averaged viscosity values at the element nodes.

Once the velocity field and flow time step have been obtained, Eqs. (3.7) and (3.10) must be solved so that the temperature profile and the degree of cure distribution are available for fluid flow computations in the subsequent time step. Notice that although the flow problem is essentially 2-D, the temperature and the degree of resin conversion vary in 3-D. This is due to the through-thickness heat transfer from the top and bottom mould walls to the resin-fibre system. The methodology used to solve for the temperature and the degree of resin conversion distributions is based on a hybrid Finite Element/Finite Difference (FE/FD) technique proposed in [45] for non-isothermal, reactive RTM simulations. This method is preferred over a complete 3-D FE methodology because of its proven efficiency [45] and the fact that it allows a simple handling of the through-thickness mesh. The latter feature is particularly useful during the secondary compression phase of the CRTM process. For a 3-D FE approach the through-thickness mesh generation can be difficult with the continuously varying cavity thickness, especially while simulating the process for a non-planar part. On the other hand, a simple adaptation of the FE/FD technique for the CRTM case permits the cavity thickness variations to be modelled in an efficient manner, even for the case of non-planar geometries. The steps involved in the technique are discussed next.

While solving Eq. (3.7) a time splitting method is used to separate it into two parts which represent the physics of the problem in the through-thickness and the in-plane directions respectively;

$$\rho \, C_p \, \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial z^2} + \varphi \, \dot{H}, \quad (3.15)$$

$$\rho \, C_p \, \frac{\partial T}{\partial t} + \rho_r \, C_{pr} \, u \cdot \nabla T = \nabla \cdot (k \nabla T). \quad (3.16)$$

In Eqs. (3.15) and (3.16) $k = k_e + k_d$, assuming scalar thermal dispersion effects. Moreover, in Eq. (3.15), where $z$ is a coordinate in the normal direction to the part surface, the convective term vanishes as the resin flows predominantly in the plane
of the part. As a result it is similar to the one dimensional Fourier’s heat conduction equation (but with an added source term) which is solved using the second-order in time, unconditionally stable Crank-Nicolson method, with the temperature of the mould walls being the boundary condition. However, this is a first approximation since the exact temperature of the mould is not known. In realistic cases temperature fluctuations are seen to occur at the mould walls, for which more general boundary conditions have been suggested in [45].

Figure 3.1: (a) Arrangement of through-thickness FD nodes at element vertices; (b) Separation of flow into identical parallel layers.

Certain factors are kept in mind while generating the through-thickness FD nodes for the Crank-Nicolson scheme. As shown in Figure 3.1a, the nodes are created exclusively at the vertex points of the triangulation used for the flow
problem. The reason for this will become apparent in subsequent discussions. Furthermore, the nodal spacing is kept uniform at all times and equal numbers of nodes are used at every location. During every flow time step of the secondary compression phase of the CRTM process it is important to ensure that the nodal spacing is shortened uniformly and in proportion to the local reduction in cavity thickness. Maintaining the nodal spacing in this manner may be viewed as a Lagrangian approach which prevents any convective term from appearing in the through-thickness direction due to mesh deformation.

Having obtained an intermediate solution for the temperature distribution, an intermediate solution for the degree of resin conversion throughout the fluid domain is obtained by updating their nodal values by applying the fourth-order accurate Runge-Kutta scheme to Eq. (3.13). Since the update of the degree of resin conversion accounts for the source term in Eq. (3.10), the part of the chemical species transport equation that remains to be solved is,

$$\varphi \frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = 0. \quad (3.17)$$

The final temperature and cure distributions within the mould at the end of the flow time step must now be found by solving the convection-dominated PDEs given by Eqs. (3.16) and (3.17). As is well known, equations of this type pose extreme challenges to a robust and accurate numerical solution. The different stabilized Galerkin FE techniques considered in this study for tackling this issue shall be described individually in Section 3.4. The ensuing part of this section discusses aspects of the solution that are common to each technique.

For the spatial discretization the flow-mesh used for solving Eq. (3.4) is employed again, but this time with conforming linear basis functions. Conforming elements are preferred here primarily because the use of non-conforming elements would lead to a larger number of degrees of freedom, which implies a greater computational cost; this follows from the observation that the number of vertices in a triangular mesh must be less than the number of sides. Moreover, unlike the solution of the governing equation for resin flow, the conservation properties of the non-conforming element do not provide any significant advantage over conforming
elements in this case. The nodes of conforming elements are located at the triangle vertices, which is compatible with the location of the through-thickness FD nodes. As depicted in Figure 3.1b, each through-thickness FD node corresponds to an independent two dimensional FE mesh layer; each a replica of the original flow-mesh. This explains the requirement that equal numbers of FD nodes be used at every location. In effect, the flow domain is divided into several parallel laminar layers over which Eqs. (3.16) and (3.17) are independently solved. Note that laminar conditions follow from the validity requirements of Darcy's law. The resin velocity profile in each layer is assumed to be identical and equal to that obtained by the application of Darcy's law to the resin pressure distribution.

As Eq. (3.16) is convective-diffusive, i.e. it is a second order PDE although with a dominant first derivative, boundary conditions are required at both the inflow and the outflow boundaries. Clearly, the boundary conditions will be different for the resin injection phase and the secondary mould compression phase of the CRTM cycle. Observe that for the complete RTM cycle and during the injection phase of the CRTM cycle the former boundary conditions will hold. During resin injection the temperature at the inflow boundary (i.e. at the injection gates) is equal to the resin injection temperature. On the other hand, during the secondary compression phase a zero heat flux condition is applied at the closed injection gates. At the flow front, however, the boundary conditions remain the same during both phases. The temperature at the front is always assumed to be at the close downstream preform temperature. This condition is not immediately apparent. Referring again to Eq. (3.16), one finds that the velocity of the thermal front is given by,

\[ u_{\text{thermal}} = \frac{\rho_r C_{pr} \varphi}{\rho C_p} \ u_{\text{pore}} \],

(3.18)

where \( u_{\text{pore}} = \frac{u}{\varphi} \) is the actual pore velocity of the fluid. Since \( \rho_r C_{pr} \varphi / \rho C_p < 1 \) the fluid front travels faster than the thermal front. As a result the resin front temperature changes quasi-instantaneously to the close downstream preform temperature (which is approximately equal to that of the heated mould walls) [74].

While solving Eq. (3.17), which is a first order PDE, a boundary condition need only be applied at the resin injection gate. During the resin injection phase the
degree of resin cure at the injection gates remain zero as fresh resin is continually injected into the mould. During the secondary compression phase of the CRTM cycle, as the resin flux is zero at the injection gates, the degree of cure at the injection nodes remains equal to that obtained at the end of the Runge-Kutta based update.

In summary, the steps involved in the general numerical approach can be enumerated as follows:

- **Step 1**: Solve the flow problem given by Eq. (3.4) and thus obtain the resin velocity field and the flow time step.

- **Step 2**: Solve the through-thickness heat conduction equation given by Eq. (3.15), by the Crank-Nicolson method or a fully-implicit (first-order in time) scheme. In this study, the thermal time step is taken equal to the flow time step. While the fully-implicit scheme places no demands on the size of the time step, with the Crank-Nicolson method it is often desirable to maintain the grid Fourier number (described in the next section) \( \leq 1 \). This thermal time step determination scheme can be included in the solution procedure in a straightforward manner.

- **Step 3**: Update the nodal degrees of resin conversion by the fourth-order accurate Runge-Kutta integration scheme.

- **Step 4**: Solve the in-plane convective-diffusive energy equation, i.e. Eq. (3.16), using a stable convection-diffusion algorithm over each of the parallel layers.

- **Step 5**: Solve the in-plane chemical species transport equation given by Eq. (3.17) also in a layer-wise manner. This can be done using the same algorithm as in Step 4.

- **Step 6**: Repeat Steps 1-5 until mould filling is complete.

### 3.3 Finite Difference Formulations

#### 3.3.1 Through-thickness heat conduction by the Crank-Nicolson method

While applying the Crank-Nicolson scheme to solve Eq. (3.15) the material
parameters $\rho C_p$, $k$, the local cavity thickness ($h$) and the local reinforcement porosity ($\varphi$) at a node are obtained by a weighted averaging of the corresponding values within the elements connected to that node. The weights are determined by the areas of the contributing elements.

The difference equation for node $i$ (through-thickness position) at location $j$ (global in-plane position) for the $(t+1)^{th}$ time step is written as,

$$T_j^{t+1} - T_j^{t} = F_0^t j^{t+1/2} \left[ \frac{T_j^{t+1, t} + T_j^{t-1, t}}{2} \right] + \gamma_j^{t+1/2}, \tag{3.19}$$

where $F_0$ is the grid Fourier number;

$$F_0^t j^{t+1/2} = \left( \frac{k}{\rho C_p} \right)_j^{t+1/2} \frac{\Delta t}{\left( \Delta h_j^{t+1/2} \right)^2}. \tag{3.20}$$

The Fourier number is a measure of the ratio of the heat conduction to storage rate. Note that if $F_0 \gg 1$ then the left hand side of Eq. (3.19) is effectively ignored, which subsequently means that the equation artificially takes a steady-state form. However, for LCM processes the small magnitude of $k/\rho C_p$ (order $10^{-7}$) prevents this from occurring.

In Eq. (3.19) $\Delta t$ is the flow time step and $\Delta h_j$ is the nodal spacing at location $j$. A superscript of $(t+1/2)$ indicates the averaged value of a parameter over the $(t+1)^{th}$ time step; e.g.,

$$\Delta h_j^{t+1/2} = \frac{\Delta h_j^{t+1} + \Delta h_j^{t-1}}{2}. \tag{3.21}$$

Assuming that the thermal properties of the constituent materials do not vary significantly with temperature or the degree of resin conversion, any change in the parameter values over a flow time step is brought about solely due to the local reduction in cavity thickness during the secondary compression phase of the CRTM process; this in turn decreases the local reinforcement porosity which alters the average material properties, as given by Eqs. (3.8) and (3.9).

The term $\gamma$ in Eq. (3.18) accounts for the heat generated due to the resin
exothermy. It is expressed as,

$$y_j^{t+1/2} = R_{a,j} i_j \left( \frac{\phi}{\rho c_p j} \right)^{t+1/2} \Delta t H_r, \quad (3.22)$$

where $H_r$ is the heat of resin reaction. The value of $R_a$ is not averaged over the $(t+1)^{th}$ time step as doing so would make the approach nonlinear and therefore require an iterative solution strategy. The computational cost attached to such an approach is considered needless.

Once the difference equations for all the through-thickness nodes at location $j$ are assembled in the form of a tridiagonal matrix, the boundary conditions for the top and bottom nodes are applied such that,

$$T_{\text{top node}} = T_{\text{bottom node}} = T_{\text{mould wall}}. \quad (3.23)$$

Having solved the discretized equations for all $j$, the intermediate approximation of the temperature distribution for the $(t+1)^{th}$ time step is used to update the nodal cure states, as discussed next.

### 3.3.2 Runge-Kutta method for updating resin cure states

The degree of resin conversion at node $(i, j)$ is updated over the $(t+1)^{th}$ time step according to the popular fourth-order accurate Runge-Kutta method for numerical integration. The steps involved in the method are as follows,

$$\Delta \alpha_1 = R_a \left( \alpha_j^{i,t}, T_j^{i,t+1} \right) \Delta t. \quad (3.24)$$

$$\Delta \alpha_2 = R_a \left( \alpha_j^{i,t} + \frac{\Delta \alpha_1}{2}, T_j^{i,t+1} \right) \Delta t. \quad (3.25)$$

$$\Delta \alpha_3 = R_a \left( \alpha_j^{i,t} + \frac{\Delta \alpha_2}{2}, T_j^{i,t+1} \right) \Delta t. \quad (3.26)$$

$$\Delta \alpha_4 = R_a \left( \alpha_j^{i,t} + \Delta \alpha_3, T_j^{i,t+1} \right) \Delta t. \quad (3.27)$$

Finally,
\[ a_j^{t+1} = a_j^t + \frac{\Delta a_1}{6} + \frac{\Delta a_2}{3} + \frac{\Delta a_3}{3} + \frac{\Delta a_4}{6}. \] (3.28)

3.4 Optimal Galerkin FE Based Convection-Diffusion Algorithms

For reasons discussed in Chapter 2, the FD approach can immediately be considered unsuitable for modelling any in-plane phenomena. The FV technique, however, provides an algorithmically straightforward means of stabilizing the solutions to convection-dominated flow problems. Despite this fact, the FE method continues to be preferred due to its superior accuracy, which primarily results from the nodal connectivity. The cell-averaging design of the FV method can sometimes dampen the occurrence of certain physical phenomena.

As the challenges encountered in numerically solving Eqs. (3.16) and (3.17) are similar, in this section only the in-plane thermal energy transport equation, i.e. Eq. (3.16), shall be considered while describing the different convection-diffusion algorithms. The solution procedure used will be essentially the same as that which would be used for the chemical species transport equation as well.

The importance of having a numerical scheme that accurately models the non-isothermal LCM process has motivated researchers in the field of composites manufacturing to find numerical algorithms that provide a physically correct solution to the convection-diffusion problem. Although a good number of methods have been tested within the LCM setting, there is no one scheme that has been accepted as being optimal for non-isothermal LCM simulations. In [70] a non-FE method was attempted for this problem; namely a FV based modified Crank-Nicolson scheme was employed. However, while computing the convective fluxes through an element boundary, the temperature condition along the boundary was considered to be the average of the cell-centred temperatures of the elements sharing the boundary. For a 1-D case this can be seen to reduce to a central differencing of the first order spatial derivative term. Such an approach is bound to make oscillatory predictions unless an extremely fine spatial discretization is used. A mathematical proof of this fact shall be provided in Section 3.4.1. The large computation time that a fine spatial discretization entails is undesirable. Moreover, in Section 3.4.1 it shall also be shown that the classical Galerkin approach is nothing
but an FE counterpart of the central differencing FD scheme. As a result, the classical Galerkin FE method too faces the same handicap when it comes to modelling the convection-diffusion problem.

In [46] a Taylor-Galerkin formulation, which uses higher order accuracy in the temporal derivate, was considered. Although the method makes reasonably stable predictions in some cases, it is not unconditionally stable and often breaks down for more sensitive problems. For this reason the method is not explored further in this study. A mixed Galerkin/Lesaint-Raviart formulation [31] and the streamline upwind Petrov-Galerkin (SUPG) method [21] have been used in [45, 56] and [42, 43], respectively. Both these methods are known to be stable and make physically acceptable predictions of the temperature profile inside the mould cavity. However, due to the lack of monotonicity properties in their FE coefficient matrices they often lead to small over/under-shoots in the neighbourhood of sharp gradients in the temperature field. Furthermore, the Lesaint-Raviart method requires each element of the spatial discretization to be solved sequentially in an order determined by the direction of the characteristics. This ordering must be repeated in each time step, and is therefore computationally intensive.

In order to further suppress even the small oscillations occurring in the solution of the temperature field, a nonlinear FE based flux-corrected transport (FEM-FCT) methodology [29] was recently implemented in [44]. However, it may be argued that the flux limiting step of the FEM-FCT method is based on heuristic arguments rather than precisely modelling the underlying physics of the problem. Moreover, the nonlinear nature of the solution procedure renders the method computationally expensive as compared to its counterparts.

In Sections 3.4.2 - 3.4.6 detailed descriptions of the numerical algorithms which have so far proven at least partially successful in modelling the heat transfer during non-isothermal LCM process simulations are provided, albeit with occasional modifications and/or enhancements to their existing form. Additionally, two nonlinear methods, namely Beyond-SUPG (BSUPG) [34] and the Mizukami-Hughes Petrov-Galerkin (MHPG) [33] scheme, are tested in an LCM setting for the first time. In particular, the MHPG algorithm is developed to deal with unsteady processing
conditions in an efficient manner; under suitable modifications, it is found that this scheme performs very well for the type of problems under consideration.

3.4.1 Inadequacy of the classical Galerkin FE method

In order to show the difficulty faced by the classical Galerkin FE method in solving the convection-diffusion PDE, the following model problem for a one-dimensional steady-state case is considered [22],

\[
\frac{dT}{dx} = k \frac{d^2T}{dx^2} \tag{3.29}
\]

along with the following boundary conditions,

\[
T = 0 \quad \text{at} \quad x = 0 \\
T = 1 \quad \text{at} \quad x = L. \tag{3.30}
\]

The general solution to Eq. (3.29) is,

\[
T(x) = C_1 + D_1 e^{ux/k}. \tag{3.31}
\]

On applying the boundary conditions the following exact solution is obtained,

\[
T(x) = \frac{1 - e^{Pe x/L}}{1 - e^{Pe}}, \tag{3.32}
\]

where \(Pe\) is the dimensionless global Peclet number, which is defined as the ratio of convective to diffusive transport rates, and is given by,

\[
Pe = \frac{uL}{k}. \tag{3.33}
\]

While solving Eq. (3.29) by the FE method linear symmetric basis functions \((w)\) are used but in conjunction with linear asymmetric, discontinuous weighting functions, as shown in Figure 3.2. Note that the perturbation, \(+/- w_p\) where \(w_p \geq 0\), only weights the interiors of the element, and therefore does not affect the application of the natural boundary condition. Clearly, choosing the perturbation to the weighting functions to be zero, i.e. setting \(w_p = 0\), would reduce the formulation to a classical Galerkin FE scheme.
The range \([0,L]\) of \(x\) is divided into \(n\) equal elements of length \(\Delta x = L/n\), and contains a total of \(n+1\) nodes numbered by \(j\), with \(j \in [0,n]\). Under this description the general solution at the nodal points can be written as,

\[
T_j = C_1 + D_1 e^{(u \Delta x/j)}.
\] (3.34)

On applying the following weak formulation using the perturbed weights for any node \(j \in [1,n-1]\),

\[
\int_{j-1}^{j}(w + w_p)\left(u \frac{dT}{dx} - k \frac{d^2T}{dx^2}\right)dx + \int_{j}^{j+1}(w - w_p)\left(u \frac{dT}{dx} - k \frac{d^2T}{dx^2}\right)dx = 0,
\] (3.35)

the discretized equation for the \(j^{th}\) node takes the form,

\[
T_{j+1}[1 - Pe'(1 - 2w_p)] - 2T_j[1 + Pe'(2w_p)] + T_{j-1}[1 + Pe'(1 + 2w_p)] = 0.
\] (3.36)

Here \(Pe'\) is the grid Peclet number which is defined as,

\[
Pe' = \frac{u \Delta x}{2k}.
\] (3.37)

Drawing an inference from Eq. (3.34), a trial solution of the form \(T_j = \Psi j\) is assumed for Eq. (3.36). Placing this in Eq. (3.36) one finds that \(\Psi\) must satisfy the following quadratic expression,

\[
[1 - Pe'(1 - 2w_p)]\Psi^2 - 2[1 + Pe'(2w_p)]\Psi + [1 + Pe'(1 + 2w_p)] = 0.
\] (3.38)
Therefore,

\[ \psi = 1 \text{ or } \frac{1+Pe'(1+2w_p)}{1-Pe'(1-2w_p)} \]  \hspace{1cm} (3.39)

One can now write the general solution of Eq. (3.36) as,

\[ T_j = C_2 + D_2 \left\{ \frac{1+Pe'(1+2w_p)}{1-Pe'(1-2w_p)} \right\}^j \]  \hspace{1cm} (3.40)

If the term within the curly brackets is negative, the spatial approximation of \( T \) is bound to oscillate as \( j \) takes on odd and even values alternately. Therefore, considering that each individual parameter within the brackets is positive, for an oscillation-free prediction either of the following requirements must be enforced,

(i) \[ 2w_p \geq 1 \]

(ii) \[ 2w_p < 1 \text{ and } Pe' < \frac{1}{1-2w_p} \]  \hspace{1cm} (3.41)

Note that replacing \( 2w_p = 1 \) in Eq. (3.36) reduces the convective term to a backward differenced (or upwind) FD form, while replacing \( 2w_p = 0 \) reduces it to a central differenced FD form. Since \( w_p = 0 \) also implies a classical Galerkin FE method, it follows that the central differenced FD and the classical Galerkin FE methods are indeed equivalent. From the requirements stated in Eq. (3.41) it can also be concluded that an upwinding of the convective term will always lead to non-oscillatory solutions whereas the solution obtained through a classical Galerkin FE approach is certain to oscillate unless \( Pe' < 1 \) (in other words, \( \Delta x \) must be less than or equal to \( 2k/u \)). This inference has been tested on the model problem given by Eq. (3.29), by arbitrarily setting \( u = 5, k = 1 \) and \( L = 5 \). From the results depicted in Figure 3.3, it can indeed be seen that the performance of the central differenced FD scheme deteriorates with increasing grid Peclet number, whereas the backward differenced scheme remains robust and oscillation free. The grid Peclet number is increased by progressively increasing \( \Delta x \), i.e. progressively using a coarser mesh. Since in LCM processes the convective effects are dominant, they place stringent fineness requirements on the spatial discretization if a classical Galerkin FE based
simulation approach is to be used. On the other hand, an appropriately upwinded FE formulation, i.e. with \( w_p \in (0, 0.5) \), can be used on coarser meshes.

For the 1-D case the exact amount of upwinding required can be determined by equating the forms of Eqs. (3.34) and (3.40). This leads to,

\[
    w_p = \frac{1}{2} \left( \coth P e' - \frac{1}{P e'} \right).
\]

(3.42)

This strategy of applying perturbations to the FE weighting functions such that it results in an accurate upwinding scheme is one that will be used in many of the algorithms to be discussed for obtaining stable oscillation-free solutions to the convection-diffusion PDE occurring in the 2-D surface flow case.

Figure 3.3: Deterioration in the performance of the central differenced FD scheme with increasing grid Peclet number.
3.4.2 Streamline Upwind Petrov-Galerkin (SUPG)

The SUPG method is one that utilizes the approach of perturbing the weighting functions as previously described. In multiple dimensions the perturbation can be defined in a more general form for the \(i^{th}\) node of an element as,

\[
wp_i = \tau \, u \cdot \nabla w_i. \tag{3.43}
\]

The total weighting function can then be written as,

\[
\tilde{w}_i = w_i + \tau \, u \cdot \nabla w_i. \tag{3.44}
\]

Comparing this to the 1-D case, the coefficient \(\tau\) is,

\[
\tau = \left( \frac{\Delta x}{2 |u|} \right) \left( \coth P_{e'} - \frac{1}{P_{e'}} \right). \tag{3.45}
\]

Therefore \(\tau\) has the dimensions of time and depends on element parameters such as element size and the grid Peclet number. As the description of element size is somewhat vague for 2-D problems, in [75] a formula for computing \(\tau\) for the case of linear triangular elements was suggested:

\[
\tau_i = \frac{1}{2} \left( \frac{M_{L e ii}}{\max_j |c_{e ij}| + D_{e ii}} \right), \tag{3.46}
\]

where \(M_{L e}, c_e\) and \(D_e\) are the Galerkin-type element lumped (row-summed) mass, convection and diffusion matrices respectively, while \(i\) and \(j\) denote element node numbers or the rows and columns of the matrices.

For the case of non-isothermal LCM simulations it is practical to consider \(\max_j |c_{e ij}| \gg D_{e ii}\). Therefore, \(D_{e ii}\) can be dropped from Eq. (3.46). Moreover, since \(M_{L e ii}\) for a triangular element of area \(\Delta\) is simply \(\Delta/3\) for all \(i\), \(\tau\) no longer varies between element nodes and is written as,

\[
\tau = \frac{1}{2} \left( \frac{M_{L e ii}}{\max_j |c_{e ij}|} \right), \quad \text{for any } i \in [1, 3]. \tag{3.47}
\]
This formula for $\tau$ leads to defining the element size as the maximum element dimension in the direction of $u$ [75]. Furthermore,

$$\sum_i \bar{w}_i = \sum_i w_i + \tau u \cdot (\sum_i \nabla w_i) = 1. \quad (3.48)$$

The fact that the weighting functions form a partition of unity, points to a local conservation statement [41].

In [35] a Galerkin/least-squares FE method was presented as a conceptual simplification of the SUPG. For the case of piecewise linear elements, like the ones employed herein, the method was shown to be identical to SUPG.

### 3.4.3 Beyond-SUPG (BSUPG)

In [34] a ‘discontinuity-capturing’ term was added to the definition of the weighting function;

$$\bar{w}_i = w_i + \tau_1 u \cdot \nabla w_i + \tau_2 u_{||} \cdot \nabla w_i, \quad (3.49)$$

where $u_{||}$ denotes the projection of $u$ onto $\nabla T_{\Omega_e}$ which is the gradient of the temperature field within an element $\Omega_e$.

$$u_{||} = \begin{cases} \frac{(u \cdot \nabla T_{\Omega_e})}{|\nabla T_{\Omega_e}|^2} \nabla T_{\Omega_e}, & \text{if } \nabla T_{\Omega_e} \neq 0, \\ 0, & \text{if } \nabla T_{\Omega_e} = 0. \end{cases} \quad (3.50)$$

$\tau_1$ and $\tau_2$ are determined similar to the SUPG method with $\tau_1 = \tau$ and $\tau_2 = \tau_{||}$ (i.e. $\tau$ computed by using $u_{||}$ in the Galerkin-type convection matrix). From the definition of $u_{||}$ it follows that,

$$u \cdot \nabla T_{\Omega_e} = u_{||} \cdot \nabla T_{\Omega_e}. \quad (3.51)$$

Using Eq. (3.51), the convection term in the weak form of Eq. (3.16) can be written as,
\[
\int_{\Omega_e} \tilde{w} \rho_r C_{pr} \mathbf{u} \cdot \nabla T \, d\Omega_e = \int_{\Omega_e} \rho_r C_{pr} w \mathbf{u} \cdot \nabla T \, d\Omega_e + \int_{\Omega_e} \rho_r C_{pr} (\tau_1 \mathbf{u} \cdot \nabla w) \mathbf{u} \cdot \nabla T \, d\Omega_e + \\
\int_{\Omega_e} \rho_r C_{pr} (\tau_2 \mathbf{u}_|| \cdot \nabla w) \mathbf{u}_|| \cdot \nabla T \, d\Omega_e.
\] (3.52)

The third term on the right hand side of Eq. (3.52) adds artificial diffusion in the direction of \(\nabla T\), which tends to smooth out the small oscillations that may occur in the vicinity of a steep temperature gradient while using the standard SUPG. Clearly, when \(u_|| = u\) the influence of artificial diffusion is effectively doubled. To prevent this, the following condition is introduced,

\[
\tau_2 = \max(0, \tau_|| - \tau).
\] (3.53)

The BSUPG method is essentially a nonlinear scheme as the ‘discontinuity-capturing’ term depends on the gradient of the field variable, making the method expensive in terms of CPU time. However, in this study, while computing the temperature field at the \((t+1)\text{th}\) step using an implicit backward Euler time stepping scheme, the temperature field at the \(t\text{th}\) step alone is considered while calculating \(u_||\). This is an effective way of linearizing the method under the assumption that the direction of the temperature gradient does not change appreciably during a single time step. As a result the computational cost of the method is considerably reduced.

3.4.4 Mizukami-Hughes Petrov-Galerkin (MHPG)

Although the Petrov-Galerkin schemes, i.e. those schemes in which the basis functions and the weighting functions are dissimilar, discussed so far give physically acceptable solutions (as shall be shown in Section 3.5), none of them satisfy monotonicity conditions. Thus, they do not preclude the existence of small over/under-shoots in the neighbourhood of sharp gradients in the temperature field. The MHPG method, introduced in [33], uses discontinuous weighting functions which are designed to enforce the discrete maximum principle on the solution of the steady-state convection-diffusion equation when discretized by a triangulation of weakly acute type. With some modifications the MHPG method can be extended to enforce monotonicity on the solution of the unsteady PDE governing non-isothermal LCM processes.
A matrix \( A \) is monotone if \( A^{-1} \geq 0 \) [29]. This property leads to the following inference,

\[
A \cdot X \geq 0 \implies X \geq 0.
\]  

(3.54)

Therefore a monotone scheme is *positivity-preserving*, and does not lead to any unphysical negative values in the field variable.

The following conditions are *sufficient* for a matrix \( A \) to be monotone [29],

\[
\begin{align*}
A_{ii} & > 0 \quad \forall \ i, \\
A_{ij} & \leq 0 \quad \forall \ j \neq i, \\
\sum_j A_{ij} & \geq 0 \quad \forall \ i.
\end{align*}
\]  

(3.55)

While constructing the element convection and diffusion matrices \( (C_e’ \text{ and } D_e’) \) by the MHPG method the discontinuous weighting functions are assumed to be of the form,

\[
\tilde{w}_i = w_i + w_{p_i} \quad (i = 1, 2, 3),
\]  

(3.56)

where the perturbations again depend on the direction of the \( \nabla T_{le} \) vector and are defined so as to satisfy the following constraints,

\[
\begin{align*}
w_{p_i} & \geq -\frac{1}{3} \quad \forall i, \\
\sum_i w_{p_i} & = 0,
\end{align*}
\]  

(3.57)

and the conditions stated in Eq. (3.55). Note that the latter requirement of Eq. (3.57) results in a partition of unity of the weighting functions which guarantees local conservation [41]. It is also easy to see that \( D_e’ \) is equal to \( D_e \), which is monotone when the triangulation is of the weakly acute type.

In order to meet the conditions in Eq. (3.55) the fundamental observation made is that for any vector \( \mathbf{v} \) perpendicular to \( \nabla T_{le} \) the following holds within \( \Omega_e \)

\[
\text{If } \tilde{\mathbf{u}} = \mathbf{u} + \mathbf{v}, \text{then } \tilde{\mathbf{u}} \cdot \nabla T = \mathbf{u} \cdot \nabla T.
\]  

(3.58)
Defining $C'_{eij}$ as,

$$C'_{eij} = \int_{\Omega_e} w_i \cdot \nabla w_j \, d\Omega_e,$$  \hspace{1cm} (3.59)

and $\tilde{C'}_{eij}$ as,

$$\tilde{C'}_{eij} = \int_{\Omega_e} \tilde{w}_i \cdot \nabla w_j \, d\Omega_e,$$  \hspace{1cm} (3.60)

it follows from Eq. (3.58) that,

$$\sum_{j=1}^{3} (C'_{eij} - \tilde{C'}_{eij}) T_j = \int_{\Omega_e} \tilde{w}_i (u \cdot \nabla T - \bar{u} \cdot \nabla T) \, d\Omega_e = 0.$$  \hspace{1cm} (3.61)

Therefore, since $C'_{eij}$ and $\tilde{C'}_{eij}$ are equivalent, choosing the perturbations such that the matrix $\tilde{C'}_{eij}$ satisfies Eq. (3.55) would imply $C'_{eij}$ to be monotone even without necessarily satisfying Eq. (3.55).

In order to find the required perturbation values, the element is first partitioned into vertex zones and edge zones as shown in Figure 3.4.

![Figure 3.4: Partition of an element into vertex and edge zones [33].](image)

It is assumed in further discussions, without any loss in generality, that $u$ lies either in the vertex or edge zone of node 1 (as shown in Figure 3.4). The flowchart
for obtaining the perturbations is accordingly provided in Figure 3.4. For a complete exposition of the mathematical arguments behind the steps refer to [33].

In Figure 3.5 conditions (C) and (D) require further explanation. Since apart from being perpendicular to $\nabla T_{\Omega e}$ the vector $\mathbf{v}$ is arbitrary, the vector $\bar{\mathbf{u}}$ is not uniquely defined. Through geometrical constructions it can however be shown that for (C) to hold $\partial \Omega_{e_{12}} \cdot \mathbf{u}_\parallel$ must be greater than zero, where $\partial \Omega_{e_{12}}$ is a vector pointing from node 1 to node 2 of the triangular element [33]. Similarly for (D) to hold $\partial \Omega_{e_{13}} \cdot \mathbf{u}_\parallel$ must be greater than zero, where $\partial \Omega_{e_{13}}$ is a vector pointing from node 1 to node 3 of the element. Moreover, at least one of (C) and (D) must be true once condition (B) occurs [33].

$(A) \ u \cdot \nabla w_1 > 0; \ u \cdot \nabla w_2 \leq 0; \ u \cdot \nabla w_3 \leq 0$

$(B) \ u \cdot \nabla w_1 < 0; \ u \cdot \nabla w_2 > 0; \ u \cdot \nabla w_3 > 0$

$(C)$ There exists $\bar{\mathbf{u}}$ such that $\bar{\mathbf{u}} \cdot \nabla w_1 < 0; \bar{\mathbf{u}} \cdot \nabla w_2 > 0; \bar{\mathbf{u}} \cdot \nabla w_3 < 0$

$(D)$ There exists $\bar{\mathbf{u}}$ such that $\bar{\mathbf{u}} \cdot \nabla w_1 < 0; \bar{\mathbf{u}} \cdot \nabla w_2 < 0; \bar{\mathbf{u}} \cdot \nabla w_3 > 0$

Figure 3.5: Flowchart for obtaining perturbations to the weighting functions.
Once $\mathbf{C}'$ and $\mathbf{D}'$ (the global convection and diffusion matrices) have been constructed, if they are combined with the consistent mass matrix ($\mathbf{M}_C$), they reduce Eq. (3.16) to the following semi-discrete form,

$$\mathbf{M}_C \frac{dT}{dt} + (\mathbf{C}' + \mathbf{D}')T = 0,$$

(3.62)

where the positive off-diagonal terms of $\mathbf{M}_C$ tend to disrupt monotone properties of the scheme as required by Eq. (3.55). Therefore, to maintain monotonicity of the MHPG method for the case of an unsteady problem, a row-summed lumped mass matrix must be used. The semi-discrete representation of Eq. (3.16) then takes the following final form,

$$\mathbf{M}_L \frac{dT}{dt} + (\mathbf{C}' + \mathbf{D}')T = 0.$$

(3.63)

Moreover, since,

$$\sum_{i=1}^{3} \nabla w_i = 0,$$

(3.64)

the row sums of $(\mathbf{C}' + \mathbf{D}')$ are exactly zero. Using this fact, the following expression can be obtained from Eq. (3.63) [29],

$$\mathbf{M}_L \frac{dT_i}{dt} = -\sum_{j \neq i} (\mathbf{C}' + \mathbf{D}')_{ij} (T_j - T_i).$$

(3.65)

From the monotonicity conditions and the equivalence of $\mathbf{C}'_{eij}$ and $\mathbf{C}'_{eij}$, it follows that if the maximum temperature occurs at point $i$, i.e. $T_i \geq T_j, \forall j$, then,

$$-(\mathbf{C}' + \mathbf{D}')_{ij} (T_j - T_i) \leq 0, \forall j \Rightarrow \frac{dT_i}{dt} \leq 0.$$

(3.66)

This shows that a maximum in the temperature field cannot increase and, extending the same argument, a minimum in the temperature field cannot decrease. Therefore the prediction of the temperature field obtained by the MHPG method at the $(t+1)^{th}$ time step is bounded by the maxima and minima of the temperature field at the $t^{th}$ step. This property, termed as local extremum diminishing (LED), precludes the existence of any unphysical over/under-shoots about sharp temperature gradients.
The MHPG, like BSUPG, was originally defined as a nonlinear scheme with the perturbations being dependent on the temperature gradient. However, here again, while applying the backward Euler implicit procedure for the temperature field at the \((t+1)^{th}\) time step, the linearization approach of considering the temperature field at the \(t^{th}\) step alone while computing the \(\Delta_i's\) is taken.

**3.4.5 FE method based Flux-Corrected Transport (FEM-FCT)**

A standard FCT procedure consists of the following steps [23, 24]:

- Solve the PDE using a low-order, highly diffused numerical scheme that prevents any unphysical oscillations of the field variable.

- Apply limited anti-diffusive fluxes in a manner that localizes the extra diffusion to only those regions of the field where the unphysical over/under-shoots tend to occur.

The anti-diffusive flux application is a nonlinear process which makes this method computationally costly. However, in [29], FEM-FCT algorithms with flux linearization techniques were introduced. It is this linearized version that is considered in the present study.

The low-order scheme is constructed by adding an artificial diffusion matrix \(\mathbf{D}_a\) to the classical Galerkin FE based semi-discretized form of Eq. (3.16) – with a lumped mass matrix. The construction of \(\mathbf{D}_a\) is based on imposing sufficiency conditions of monotonicity, as stated in Eq. (3.55), onto the sum of the classical Galerkin based global convection and diffusion matrices, i.e. \(\mathbf{C}\) and \(\mathbf{D}\). Moreover, \(\mathbf{D}_a\) must be symmetric with zero row and column sums, in order to ensure consistency and thermal energy conservation. Both these requirements are fulfilled by the following design [29],

\[
\mathbf{D}_{a_{ii}} = -\sum_{j \neq i} \mathbf{D}_{a_{ij}} \text{ with } \mathbf{D}_{a_{ij}} = \mathbf{D}_{a_{ji}} = \min\{0, -(\mathbf{C} + \mathbf{D})_{ij}, -(\mathbf{C} + \mathbf{D})_{ji}\}. \tag{3.67}
\]

On adding a limited anti-diffusive flux vector \(\mathbf{F}\) to the low-order scheme, it takes the following semi-discrete form,
The first step towards obtaining the vector $F$ is to calculate the raw inter-nodal fluxes ($F_{ij}$). This is done by first approximating the temperature field at the $(t+1)^{th}$ step using a higher order scheme for Eq. (3.16) (the classical Galerkin FE – with a consistent mass matrix) and then applying the following prescription [29];

$$F_{ij} = \left[ \frac{M_{ij}(T_{i}^{t+1} - T_{j}^{t+1}) - M_{ij}(T_{i}^{t} - T_{j}^{t})}{\Delta t} \right] - D_{ij}(T_{i}^{t+1} - T_{j}^{t+1}). \quad (3.69)$$

(Note that Eq. (3.69) corresponds to the implicit backward Euler time stepping scheme. For a full description on obtaining the inter-nodal fluxes when using other time stepping schemes, refer to [29].) Finally,

$$F_i = \sum_{j \neq i} \alpha_{ij} F_{ij}, \quad (3.70)$$

where $\alpha_{ij} \in [0,1]$ are correction factors obtained by Zalesak’s algorithm [25]. The steps involved in the algorithm are as follows [29]:

- **Step 1:** Compute the total flux flowing into and the total flux flowing out of node $i$.

$$P_i^+ = \sum_{j \neq i} \max\{0, F_{ij}\}; \quad P_i^- = \sum_{j \neq i} \min\{0, F_{ij}\}. \quad (3.71)$$

- **Step 2:** Compute the distance between the nodal solution at $i$ and a local extremum at time step $t$.

$$S_i^+ = \max\{0, \max_{j \neq i}(T_{i}^{t} - T_{j}^{t})\}; \quad S_i^- = \min_{j \neq i}\{0, \min(T_{j}^{t} - T_{i}^{t})\}. \quad (3.72)$$

- **Step 3:** Compute correction factors for node $i$.

$$R_i^+ = \min\left\{1, \frac{M_{ij}S_i^+}{\Delta t P_i^+} \right\}; \quad R_i^- = \min\left\{1, \frac{M_{ij}S_i^-}{\Delta t P_i^-} \right\}. \quad (3.73)$$

- **Step 4:** Compute $\alpha_{ij}$.
\[ \alpha_{ij} = \begin{cases} \min\{R_i^+, R_j^-\} & \text{if } F_{ij} > 0 \\ \min\{R_i^-, R_j^+\} & \text{otherwise} \end{cases} \quad \text{(3.74)} \]

This flux limiting strategy ensures that the temperature field at the \((t+1)\)th step is bounded by the maxima and minima of the temperature field at the \(t\)th step. This can be proven by first rewriting Eq. (3.68) as,

\[ \frac{M_L}{\Delta t} T^{t+1} + (C + D + D_a) T^{t+1} = \frac{M_L}{\Delta t} T^t + F. \quad \text{(3.75)} \]

Assume that there exists some '\(i\)' such that \(T_{t+1}^{i} = \max_j \{T_{j}^{t+1}\} > \max_j \{T_{j}^{t}\}\). From the limiting strategy it follows that,

\[ \frac{M_{li}}{\Delta t} T_{i}^t + F_{i} \leq \frac{M_{li}}{\Delta t} \max_j \{T_{j}^{t}\}. \quad \text{(3.76)} \]

On the other hand, the monotone property of the matrix \((C + D + D_a)\) leads to,

\[ \frac{M_{li}}{\Delta t} \max_j \{T_{i}^{t}\} < \frac{M_{li}}{\Delta t} T_{i}^{t+1} + \sum_j (C + D + D_a)_{ij} T_{j}^{t+1}, \quad \text{(3.77)} \]

which together with Eq. (3.76) violates the equality of Eq. (3.75). Therefore, since the assumption leads to a contradiction, it can never happen that the maximum temperature at the \((t+1)\)th step exceeds that at the \(t\)th step. A similar argument can be used to prove the lower bound of the temperature field as well.

Even though Zalesak’s algorithm keeps the temperature profile bounded, in [76] it has been demonstrated that Zalesak’s flux limiter does not prevent the creation of new and the enhancement of existing numerical ripples in the case of multidimensional problems, i.e. the limiter is positivity-preserving but not monotone. The ramification of this fact shall be revealed while testing the numerical scheme.

\textbf{3.4.6 Mixed Galerkin /Lesaint-Raviart}

This method involves further splitting Eq. (3.16) into two parts which deal with diffusion and transport separately [45];
\[ \rho \, C_p \, \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T), \quad (3.78) \]

\[ \rho \, C_p \, \frac{\partial T}{\partial t} + \rho_r \, C_{pr} \, \mathbf{u} \cdot \nabla T = 0. \quad (3.79) \]

Eq. (3.78), representing in-plane diffusion, is solved using the classical Galerkin FE technique, while Eq. (3.79) is solved with the Lesaint-Raviart transport approximation. The Lesaint-Raviart approximation, originally developed in [30], is essentially a Discontinuous Galerkin (DG) method in which the element nodes lying on the triangle vertices are thought of as actually lying within the interiors of the triangles but arbitrarily close to the vertices [30]. Therefore no \( C_0 \) continuity requirements are imposed anywhere along element boundaries, a feature which allows the DG method to efficiently resolve steep gradients in the temperature field.

The approximate solution over an element \( \Omega_e \) is obtained by solving the following weak formulation derived from Eq. (3.79):

\[ \int_{\Omega_e} \int_{\Omega_e} w \rho C_p \, \frac{\partial T}{\partial t} \, d\Omega_e + \int_{\partial \Omega_e} w \rho_r C_{pr} \, \mathbf{u} \cdot \nabla T \, d\partial \Omega_e = \int_{\partial \Omega_e} \rho_r C_{pr} (T^+ - T^-) w^+ \mathbf{u} \cdot \mathbf{v} \, dl. \quad (3.80) \]

The right hand side of the equation is a Dirac delta function at the inflow boundaries \( (\partial \Omega_e) \) due to the jump discontinuity at these boundaries. The scalar parameter \( \xi^{+/-} \) is defined as follows:

\[ \xi^+(x) = \lim_{\epsilon \to 0^+} \xi(x + \epsilon \mathbf{u}); \quad \xi^-(x) = \lim_{\epsilon \to 0^-} \xi(x + \epsilon \mathbf{u}), \quad (3.81) \]

where \( x \) is a point in the flow domain.

An implicit backward Euler time stepping is used for the temporal derivative in Eq. (3.80). This requires that prior to solving Eq. (3.80) for a particular element, the equation must have already been solved on all elements sharing its inflow boundaries. This is achieved by starting the solution with elements adjacent to the injection port, then sweeping through the complete flow domain in an order determined by the direction of the characteristics. In general the ordering must be repeated in every time step and can be prohibitively expensive in the case of complex geometries modelled with a fine unstructured mesh. For an efficient
sweeping algorithm it is proposed here to use the fast nondominated sorting approach of the Nondominated Sorting Genetic Algorithm II (NSGA-II) [59], based on a definition of nondomination which is specifically adapted for the transport problem. For each element in the flow mesh two entities are computed: 1) the number of elements sharing its inflow boundaries \(n_e\), which are considered to be the elements that dominate the present one, and 2) the set of elements sharing its outflow boundaries \(S_e\), which are considered to be the elements dominated by the present one. Following this computation, the fast nondominated sort algorithm technique, which shall be discussed in detail in Part 2 of this thesis, is used to rank (order) the elements. Note that the algorithm may not work if the flow contains vortices.

Due to the use of linear basis functions, the fluid velocity field obtained from Darcy’s law is always uniform over an element. This violates continuity conditions within the element during the secondary compression phase of the CRTM process, when the velocity field must be divergent at every point in the flow domain. Therefore, it is inaccurate to consider the resin velocity within an element to be uniform while solving Eq. (3.80) during this phase. In order to improve the performance it is proposed here to use a device introduced in [77, 78]. The velocity \(\mathbf{u}\) is first approximated over an element by the linear function \(\mathbf{u}_a\) using a Taylor series expansion about the barycentre \(x_b\) of the element,

\[
\mathbf{u}_a(x) = \mathbf{u}_a(x_b) + \frac{\partial \mathbf{u}}{\partial x = x_b} (x - x_b), \quad x \in \Omega_e. \tag{3.82}
\]

Assuming that \(\mathbf{u}_a\) varies over the element according to,

\[
\mathbf{u}_a(x) = \begin{pmatrix} c_1 + c_2 x \\ c_3 + c_2 y \end{pmatrix}, \tag{3.83}
\]

then,

\[
\frac{\partial \mathbf{u}}{\partial x = x_b} (x - x_b) = c_2 (x - x_b) = \frac{1}{2} (\nabla \cdot \mathbf{u}_a) (x - x_b). \tag{3.84}
\]

Since the mould cavity thickness is assumed to be more-or-less uniform over the element, the following can be said from Eq. (2.1),
\[ \nabla \cdot \mathbf{u}_a = - \frac{1}{h} \frac{\partial h}{\partial t}. \]  
(3.85)

Substituting Eqs. (3.84) and (3.85) into Eq. (3.82), one has,

\[ \mathbf{u}_a(x) = \mathbf{u}_a(x_b) - \frac{1}{2} \frac{1}{h} \frac{\partial h}{\partial t} (x - x_b). \]  
(3.86)

Finally, assuming that the velocity at the barycentre is equal to the original approximation from Darcy’s law, one obtains the velocity field within the element in its final form;

\[ \mathbf{u}_a(x) = \frac{\mathbf{K}}{\mu} \nabla p_{De} - \frac{11}{2h} \frac{\partial h}{\partial t} (x - x_b), \quad x \in \Omega_e. \]  
(3.87)

Eq. (3.87) can be substituted into the boundary integral term of the DG weak formulation to improve its physical accuracy. Also observe that since,

\[ \int_{\partial \Omega_{e_i}} \frac{1}{2h} \frac{\partial h}{\partial t} (x - x_b) \cdot \mathbf{v} \, hdl = \frac{\partial h}{\partial t} \frac{\Delta t}{3}, \]  
(3.88)

the resin discharge through side \( \partial \Omega_{e_i} \) obtained via the linear approximation of the velocity field is indeed consistent with that obtained through the non-conforming FE approach; see Eq. (2.22). Moreover, with the proposed enhancement, the DG method becomes the only one, among all the tested algorithms, that explicitly models the divergence in the fluid velocity field while solving Eq. (3.16) during the secondary compression phase of the CRTM process.

**3.4.6.1 Slope limited DG method**

The Lesaint-Raviart approximation is again a method which often leads to small oscillations in the vicinity of sharp gradients in the temperature field. In order to effectively suppress oscillations for DG methods a vertex-based slope limiting strategy was developed in [40]. The strategy was described as a vertex-based counterpart of the popular Barth-Jespersen limiter [39].

The slope limiting step is essentially a postprocessing filter that enforces the nodal temperatures to remain within certain bounds [40]. The bounds for the \( i^{th} \) node, i.e. \( T_i^{\text{max}} \) and \( T_i^{\text{min}} \), are determined by the maximum and minimum
barycentric temperatures among all the elements containing node \( i \). These bounds are met by introducing a correction factor \( \alpha_\varepsilon \in [0,1] \) to the temperature gradient, which results in a reconstruction of the temperature field within the element of the form,

\[
T(x) = T(x_b) + \alpha_\varepsilon \nabla T \cdot (x - x_b) \quad x \in \Omega_e.
\] (3.89)

Note that due to the choice of linear basis functions one has,

\[
\int_{\Omega_e} \alpha_\varepsilon \nabla T \cdot (x - x_b) \, d\Omega_e = 0.
\] (3.90)

Therefore,

\[
\int_{\Omega_e} \rho c_p T(x) (\Delta h) \, d\Omega_e = \int_{\Omega_e} \rho c_p T(x_b) (\Delta h) \, d\Omega_e.
\] (3.91)

The absence of \( \alpha_\varepsilon \) in Eq. (3.91) implies that the thermal energy contained within the element is not affected by the reconstruction of the temperature field. Therefore the slope limiting strategy does not interfere with the local conservation property of the DG method.

The element-wise correction factors are obtained according to the following [40],

\[
\alpha_\varepsilon = \min_i \begin{cases}
\min \left( 1, \frac{T_{i,\max} - T(x_b)}{T_i - T(x_b)} \right), & \text{if } T_i - T(x_b) > 0, \\
1, & \text{if } T_i - T(x_b) = 0, \\
\min \left( 1, \frac{T_{i,\min} - T(x_b)}{T_i - T(x_b)} \right), & \text{if } T_i - T(x_b) < 0.
\end{cases}
\] (3.92)

### 3.5 Verification and Comparison of Numerical Schemes

The experimental scenarios considered for the comparison study, while having rather intuitive outcomes, are difficult to model by conventional numerical schemes. Moreover, reasonable analytical solutions can be derived for them. This allows rigorous verification of the predictions made by each of the transport-diffusion algorithms.
3.5.1 Experimental Case 1 (EXP 1) - Rectangular Mould Filling

Non-isothermal unidirectional mould filling experiments were carried out by Chiu et al. [58], using Palatino oil as the test fluid. The data for these experiments and the corresponding results have been obtained from [43]. The rectangular mould was 21 cm long \((L)\), 7.63 cm wide \((W)\) and had a cavity thickness of 0.8 cm \((H)\), which was packed with four layers of continuous random glass-fibre mat. The properties of the reinforcement material and the Palatino oil are given in Table 3.1 [43]. The test fluid was injected at a constant flow rate into the mould, the walls of which were preheated and held at a constant temperature of 63°C. The fluid itself was maintained at an injection temperature of 34.5°C. Its viscosity was described as a function of its temperature according to the following relation;

\[
\mu = 0.001e^{\left(\frac{44852}{T} - 11.3\right)}, \tag{3.93}
\]

where the units of \(\mu\) and \(T\) are Pa s and Kelvin, respectively.

During the experiment the test fluid was continuously injected for an additional duration, post complete filling of the mould. The temperature recordings were collected over this time as well. Figure 3.6 depicts the experimentally obtained temperature histories at three locations along the mid surface of the mould cavity, i.e. at 0.25\(L\), 0.5\(L\) and 0.75\(L\) from the injection port. It can be observed that the temperatures at the two locations nearer to the injection port reach a steady-state, whereas the temperature at the third location, although still transient, tends to a steady-state as well. It can be inferred that continuously injecting the test fluid for a sufficiently large period of time would lead to fully developed steady thermal conditions throughout the mould cavity.

| Table 3.1: Material properties for EXP 1 [43]. |
|------------------|------------------|
|                  | Palatino Oil     | Glass-fibre mat |
| \(\rho\) (g/cm\(^3\)) | 0.98             | 2.53            |
| \(C_p\) (J/g K)   | 1.88             | 0.68            |
| \(k\) (W/m K)     | 0.136            | 0.417           |
| Porosity \(\varphi\) | 0.91            |                 |
| \(K\) (m\(^2\))  | 4.8361 x 10\(^{-9}\) |                 |
3.5.1.1 Analytical Solution

In this section we derive a complete analytical solution of the 1-D form of Eq. (3.7), for the temperature profile within the rectangular part once steady-state is reached. This analytical solution will later be used to verify the numerical schemes. Without the temporal derivative term the equation can be written as,

$$\frac{\rho c_p r Q}{k H W} \frac{\partial \hat{T}}{\partial \hat{x}} - \frac{\partial^2 \hat{T}}{\partial \hat{x}^2} = \frac{\partial^2 \hat{T}}{\partial \hat{z}^2},$$

(3.94)

where \( Q \) is the constant fluid flow rate and \( \hat{T} \) is the dimensionless temperature, given by,

$$\hat{T} = \frac{T - T_{\text{min}}}{T_{\text{max}} - T_{\text{min}}}. \quad (3.95)$$

Non-dimensionalizing the space variables as,

$$\hat{x} = \frac{x}{L}, \quad \hat{z} = \frac{z}{H}, \quad (3.96)$$

Eq. (3.94) becomes,

$$\frac{\rho c_p r Q}{k H W} \left( \frac{L}{H} \right) \frac{\partial \hat{T}}{\partial \hat{x}} - \frac{\partial^2 \hat{T}}{\partial \hat{x}^2} = \left( \frac{L}{H} \right)^2 \frac{\partial^2 \hat{T}}{\partial \hat{z}^2}. \quad (3.97)$$
The magnitudes of the coefficients occurring in Eq. (3.97) suggest that for the problem under consideration the in-plane conduction term can be safely ignored. However, we hold on to this term in subsequent derivations for greater generality. Continuing with Eq. (3.94) and applying the variable separation method, the general solution for the dimensionless temperature is found to be,

$$
\hat{T} = 1 + \sum_{n=1}^{\infty} \left( c_1^ne^{\lambda_1^nx} + c_2^ne^{\lambda_2^nx} \right) \sin \frac{n\pi x}{H},
$$

(3.98)

where $c_1^n$ and $c_2^n$ are evaluated from the Fourier expansions of the boundary conditions, i.e. resin injection temperature at the inlet and mould wall temperature near the vent, while $\lambda_1^n$ and $\lambda_2^n$ are the roots of the following characteristic equation,

$$
\lambda^2 - \left( \frac{\rho c_p q}{k H W} \right) \lambda - \frac{n^2 \pi^2}{H^2} = 0.
$$

(3.99)

### 3.5.2 Experimental Case 2 (EXP 2) - Circular Mould Filling

Lin et al. [57] conducted non-isothermal mould filling experiments by injecting Palatino oil into a circular mould cavity containing random glass-fibre reinforcements. The inner radius of the mould was 0.635 cm ($R_i$), the outer radius was 20 cm ($R_o$) and the cavity thickness was 1.27 cm ($H$). The properties of the Palatino oil and the reinforcements for this second case are given in Table 3.2 [57]. The test fluid was injected at a temperature of 20°C and at a constant flow rate of 34 cm³/s. The mould walls were preheated and maintained at a constant temperature of 75°C. The thermal dependence of the fluid viscosity was expressed as follows,

$$
\mu = e^{\left( \frac{4125}{T} - 16.376 \right)}.
$$

(3.100)

<table>
<thead>
<tr>
<th>Table 3.2: Material properties for EXP 2 [57].</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Palatino Oil</strong></td>
</tr>
<tr>
<td>$\rho$ (g/cm³)</td>
</tr>
<tr>
<td>$C_p$ (J/g K)</td>
</tr>
<tr>
<td>$k$ (W/m K)</td>
</tr>
<tr>
<td>Porosity $\phi$</td>
</tr>
<tr>
<td>$K$ (m²)</td>
</tr>
</tbody>
</table>
Figure 3.7: Experimental observations for thermal histories for EXP 2; (a) at location 1 and (b) at location 2.

Figure 3.7 depicts the experimentally observed temperature histories at two locations within the mould (location 1 being 4 cm and location 2 being 8 cm away from the injection port, midway through the thickness). In this case the temperatures at both the reference points reach a steady-state condition by the time the mould gets completely filled. A third location is included (location 3 – 12 cm from the injection port) at which experimental data is not available but an analytical solution can be obtained under steady thermal conditions.

3.5.2.1 Analytical Solution

Eliminating the temporal derivative, Eq. (3.7) takes the following form in a cylindrical coordinate system,

\[
\frac{1}{\rho r c_p r} \left( \frac{\partial^2 \phi}{\partial r^2} - \frac{1}{2\pi H k} \frac{\partial \phi}{\partial r} \right) - \frac{\partial^2 \phi}{\partial z^2} = \frac{\partial^2 \phi}{\partial z^2}. \tag{3.101}
\]

Here again, although a simple scaling analysis suggests that the in-plane conduction effects will be relatively small, it is retained while deriving the general solution of Eq. (3.101). On applying the variable separation method as in the previous case, the variable varying with radial position \(r\) is required to solve the following ordinary differential equation,

\[
\frac{\partial^2 T_r}{\partial r^2} - \frac{1}{r} \left( \frac{\rho r c_p r Q}{2\pi H k} - 1 \right) \frac{\partial T_r}{\partial r} - \frac{n^2\pi^2}{H^2} T_r = 0. \tag{3.102}
\]
Considering the function,

$$\hat{T}_r = r^\gamma I_m(\beta r), \quad (3.103)$$

where $I_m(r)$ is the modified Bessel function of the first kind, $\hat{T}_r$ solves the following transformation of the modified Bessel differential equation (the derivation of this result is provided in Appendix A.1),

$$\frac{\partial^2 \hat{T}_r}{\partial r^2} - \frac{1}{r} (2\gamma - 1) \frac{\partial \hat{T}_r}{\partial r} - \left(\beta^2 + \frac{m^2 - \gamma^2}{r^2}\right) \hat{T}_r = 0. \quad (3.104)$$

Substituting,

$$\gamma = \frac{1}{2} \frac{\rho c_p Q}{\pi h \kappa}, \quad \beta = \frac{n\pi}{H}, \quad m = \gamma, \quad (3.105)$$

it is observed that Eq. (3.102) exactly resembles the transformed modified Bessel differential equation. Therefore, the general solution of Eq. (3.101) takes the form;

$$\hat{T} = 1 + \sum_{n=1}^{\infty} r^{\gamma} \left\{ c_1^n I_\gamma \left(\frac{n\pi}{H} r\right) + c_2^n K_\gamma \left(\frac{n\pi}{H} r\right) \right\} \sin \frac{n\pi z}{H}, \quad (3.106)$$

where $K_m(r)$ is the modified Bessel function of the second kind. The coefficients $c_1^n$ and $c_2^n$ are again evaluated by the Fourier expansions of the thermal boundary conditions at the injection port and the vent. It should be noted that while computing the temperature profile using Eq. (3.106), the large value of $\gamma$ for the present test case requires uniform asymptotic expansions for large orders of the modified Bessel functions, which can be found in [79].

### 3.5.3 Numerical Simulations

The finite element meshes used for the two test problems are depicted in Figure 3.8. Additionally, for both cases, 11 FD nodes are used for the through-thickness discretization. Although the experiments are truly 1-D (or axisymmetric) fluid flows, they are simulated as general 2-D flow problems. Rather coarse in-plane discretization allows suitable testing of the robustness of the stabilized convection-
diffusion algorithms. Moreover, in order to study the effect of the grid Fourier number a through-thickness mesh refinement study for the circular part is presented in Appendix A.2. The results indicate that for the problems under consideration, the quality of the simulation is not sensitive to the magnitude of Fo.

![Figure 3.8: Unstructured triangular finite element mesh for (a) EXP 1 and (b) EXP 2. Note that the figures are not in proportion.](image)

In subsequent discussions, the convection-diffusion algorithms which are known not to be positivity-preserving (i.e. Mixed Galerkin/Lesaint-Raviart, SUPG and BSUPG) will be collectively referred to as *Type 1* algorithms while those which have been designed to maintain positivity conditions (i.e. MHPG, FEM-FCT and Mixed Galerkin/slope limited DG) will be termed *Type 2* algorithms. For clarity, results and discussions pertaining to separate *types* will be presented separately.

Figure 3.9 compares the results obtained through *Type 1* algorithms for the temperature evolution at the three reference points, during EXP 1. Although the numerical predictions show reasonable agreement with the experimental
observation, the lack of positivity-preservation leads to under-shoots in the prediction of thermal histories, just prior to the onset of the steady-state condition. This under-shoot is more prominent for the Mixed Galerkin/Lesaint-Raviart scheme as compared to both SUPG and BSUPG, which practically replicate each other. Moreover, the local temperature predicted by the Mixed-Galerkin/Lesaint-Raviart scheme is seen to drop below 34.5°C, which is physically impossible given that a colder fluid (34.5°C) is injected into a heated mould. Additionally, at the final reference point (0.75L), the steady-state temperature predicted by the Mixed Galerkin/Lesaint-Raviart is significantly lower than that predicted by SUPG and BSUPG, which in turn is lower than what the experiments seem to suggest.

In Figure 3.10, which is obtained by allowing fluid flow to continue till steady-state conditions are fully developed throughout the cavity, the through-thickness temperature profiles obtained by SUPG and BSUPG agree very closely with the analytical solutions derived earlier at each of the three reference points. This feature suggests that the difference in the experimental observation and the numerical prediction at the final reference point may be a result of inherent experimental variability. Moreover, it validates the hybrid FE/FD technique in which the transport-diffusion algorithm is applied independently to separate parallel flow layers. The comparatively poor performance of the Mixed Galerkin/Lesaint-Raviart scheme may be attributed to the further splitting of Eq. (3.16), which, as the results show, is not a sufficiently diffusive simplification.
Figure 3.11 corresponds to the application of Type 2 algorithms to EXP 1. Herein the consequences of Zalesak’s algorithm not being monotone are unquestionably revealed. Low amplitude numerical ripples are observed in the temperature histories obtained through the FEM-FCT method, which tend to propagate instead of dying out instantly like in the case of Type 1 algorithms. It can also be seen that the slope limitation step added to the DG method successfully suppresses the undershoots, but the method continues to be insufficiently diffusive. The MHPG method, on the other hand, makes completely oscillation/ripple free predictions which match the experimental observations better than any of the other methods. In terms of the through-thickness temperature profiles, Figure 3.12 shows that apart from the slope limited DG method the other Type 2 algorithms are accurate.
While testing Type 1 algorithms on EXP 2, even the SUPG and BSUPG methods lead to significant under-shoots in the temperature evolution curves, as depicted in Figure 3.13. It is also interesting to note that the additional computations involved in the BSUPG method provide no improvements in numerical predictions as compared to the SUPG method, at least for neither of the two scenarios being studied. In Figure 3.14, the through-thickness thermal profiles obtained by the Type 1 schemes are, in general, in good agreement with analytical estimates. The Mixed Galerkin/Lesaint-Raviart scheme performs well at locations 1 and 2, but its accuracy deteriorates marginally at location 3.
Figure 3.14: Comparison of analytical and Type 1 numerical predictions for through-thickness temperature profiles at reference points of EXP 2.

All three Type 2 algorithms simulate EXP 2 accurately, as shown in Figures 3.15 and 3.16. Although in this case the FEM-FCT method does not show any numerical ripples, the sharp/sudden change observed in the slope of the thermal curve, in Figure 3.15, just prior to the steady condition, may be considered unphysical. The slope limited DG method is seen to perform very well in terms of completely eliminating oscillatory behaviour. The MHPG method continues to make smooth and physically realistic predictions that are closer to the experimental observations than all the other schemes tested.

Figure 3.15: Numerical simulations using Type 2 algorithms, at the two reference points in EXP 2.
Figure 3.16: Comparison of analytical and Type 2 numerical predictions for through-thickness temperature profiles at reference points of EXP 2.

3.5.4 Discussion

A group of MATLAB codes were developed to implement each of the algorithms presented in this chapter. The through-thickness heat conduction equation, i.e. Eq. (3.15), was solved independently at each node, and the in-plane convection-diffusion problem was split into independent parallel layers. This structure makes the general numerical approach highly amenable to parallel computation. However, the Parallel Computing Toolbox within MATLAB was not utilized in order to measure the performance of the algorithms when carried out on a simple, serial computer. The comparisons of the numerical simulations with the analytical solutions validate the general numerical approach by showing that the application of the convection-diffusion algorithm independently to each layer does not disrupt the through-thickness temperature profile.

On examining the Type 1 algorithms it is found that although they show acceptable stability, without generating large numerical oscillations in the temperature field, there exist small amplitude oscillations in the neighbourhood of steep gradients in the temperature field. This is to be expected as the construction of the algorithms does not take into account monotonicity conditions. The Type 2 algorithms, on the other hand, are specifically constructed by taking the monotonicity requirements into consideration, and are expected to provide completely oscillation free simulations. For the FEM-FCT algorithm, however, the implementation of a flux limiting step which is not monotone disrupts the
monotonicity satisfying conditions, leading to the existence of numerical ripples in
the simulation of one of the test cases. The slope limiting strategy applied to the DG
method does suppress the oscillation occurring in the Lesain-Raviart approach, but
retains the property of lacking the required amount of diffusion. In contrast, the
MHPG method, which has been implemented together with a lumped mass matrix
to maintain its monotonicity properties, successfully makes physically accurate,
oscillation-free predictions which are in excellent agreement with the experimental
as well as analytical data.

Table 3.3 provides a comparison of the average runtimes of the present
implementations of the different algorithms while simulating the test cases under
consideration. The SUPG method, not surprisingly, is found to be computationally
most efficient, while the FEM-FCT scheme is the most expensive and by a
substantial margin. The BSUPG method, which requires larger computations than
the SUPG, not only consumes extra computational resources, but fails to make any
significant improvement in the quality of predictions. The Mixed Galerkin/Lesaint-
Raviart and the linearized MHPG algorithms have similar runtimes, second only to
the SUPG method. However, for part geometries of greater complexity, the
repetitive calls on the characteristic direction based sweeping algorithm (an
efficient implementation of which is in itself not a trivial task) makes the Mixed
Galerkin/Lesaint-Raviart a potentially expensive choice. The reconstruction step of
the slope limiting strategy while enhancing the accuracy of the Lesaint-Raviart
method also increases the runtime of the algorithm. However, it should be noted
here that the element-wise solution approach of the DG method allows further code
parallelization, over and above that permitted by the general numerical approach.

Table 3.3: Average runtime comparison of simulations using different convection-diffusion
algorithms.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>((\text{Avg. runtime})/(\text{Avg. runtime})_{\text{SUPG}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>SUPG</td>
<td>1</td>
</tr>
<tr>
<td>BSUPG</td>
<td>2.46</td>
</tr>
<tr>
<td>MHPG</td>
<td>1.53</td>
</tr>
<tr>
<td>FEM-FCT</td>
<td>3.7</td>
</tr>
<tr>
<td>Mixed-Galerkin/Lesaint-Raviart</td>
<td>1.68</td>
</tr>
<tr>
<td>Slope Limited DG</td>
<td>2.56</td>
</tr>
</tbody>
</table>
Overall, the MHPG method proves to be very well suited for non-isothermal LCM simulations. However, its application is presently restricted to the simulation of relatively thin composite part manufacturing. For the less common case of thick part manufacturing, wherein the through-thickness flow is significant and a 3-D FE approach is unavoidable, the MHPG can no longer be used in its present form. This is because the extension of the algorithm to different element types or to higher dimensions is not immediately apparent [34]. Preliminary steps towards the construction of an algorithm which retains the features of the MHPG scheme in 3-D have been undertaken in [80].

Despite the superior accuracy of the MHPG scheme, the SUPG method has been used as the fundamental convection-diffusion algorithm throughout the study. This is primarily due to the significant saving in computational cost, which is crucial when an algorithm is to be used within a population-based search strategy for optimization. The accuracy of the SUPG scheme when applied to simulating the manufacturing process of a non-planar part has also been verified against analytically derived solutions. Since experimental results for this case are not available, the validation study has instead been provided in Appendix A.3.

3.6 Summary

In this chapter the governing equations of resin flow have been extended to include the effects of temperature and cure during non-isothermal LCM processes. A hybrid FE/FD scheme has been described which decouples the physics in the in-plane and through-thickness directions. Following this, a group of convection-diffusion algorithms were introduced and verified on a set of experimental test cases for which analytical solutions were also obtained. The comparison results show that the decoupling approach does not disrupt the through-thickness temperature variation, thereby validating its use in this research. Moreover, it is found that the Mizukami-Hughes Petrov-Galerkin (MHPG) method is most accurate for predicting thermal conditions during non-isothermal, thin-part manufacturing processes. However, the comparatively low computational cost of the streamline upwind Petrov-Galerkin (SUPG) scheme, while maintaining acceptable accuracy, has led to this method being adopted as the standard algorithm in the entire study.
Chapter 4

Simulating the Effect of Temperature Elevation on Clamping Force Requirements

The moulds used for rigid-tool LCM processes are often subjected to large internal forces which originate from the high resin injection pressure as well as the compression of the fibrous reinforcement. In this chapter, the simulation tool, described in Chapters 2 and 3, is employed in conjunction with a mixed-elastic fibre compaction model in order to predict the evolution of the internal forces acting on the mould walls during non-isothermal LCM processes, considering different combinations of the design variables. The simulations are carried out for a planar circular part and a non-planar hemispherical part. The results reveal a rather counter-intuitive effect of resin and mould temperature elevation during the resin injection phase. Moreover, they highlight the importance of the simulation tool in terms of designing an optimized manufacturing cycle, one which minimizes cycle time as well as equipment setup costs.

4.1 Fibre Compaction Model

As has been stated in the introduction, an accurate prediction of the tooling forces cannot be made without a compaction model that captures the stress-strain relation of the fibrous reinforcement when subjected to compacting loads. A variety of models have been proposed in the literature for this purpose. The most common approach among these has been to assume that the deformation occurs in a non-linear elastic manner [14, 15], with the non-linearity originating from a stiffening of the reinforcement with an increase in strain. However, experimental observations have shown the existence of deformation-rate dependency in their response, as well as the occurrence of permanent deformation of the reinforcement. These features indicate that the fibrous reinforcement truly responds in a manner that can only be defined as a combination of nonlinearity, viscoelasticity and rate-independent plasticity [81]. Modelling the plastic behaviour, however, is considered to be critical only while simulating processes which subject the reinforcement to cyclic loading; these include flexible-tool LCM processes like RTM-light and Vacuum Assisted Resin
Infusion (VARI) [81]. This is because in such cases the hysteresis effect during the unloading cycle plays an important role in determining properties such as the final part thickness and the final fibre volume fraction [81]. Since in this research only rigid-tool LCM processes are considered, for which the reinforcement undergoes only a single compaction loading, the rate-independent plastic behaviour is ignored. However, the secondary mould compression phase of the CRTM cycle makes it crucial to accurately model the strain-rate dependency. Models incorporating this effect include, (1) a nonlinear mixed-elastic model [1, 2, 12, 13], which does not make explicit use of the compression velocity even while accounting for the dynamic mould, and (2) a complete viscoelastic model [1, 2, 16-18], which explicitly takes the compression velocity into account by assuming that different stress-strain curves, i.e. for different compression speeds, collapse to a single master function when scaled [17]. Between these two models, the mixed-elastic allows the material characterisation to be carried out in a simpler manner. Moreover, the simplicity of its mathematical expression, as shall be shown in the next section, leads to superior computational efficiency, while making accurate force predictions for a variety of rigid-tool LCM simulations [2]. As a result, the mixed-elastic model has been adopted as the standard fibre compaction model throughout this research.

For tooling force predictions in the case of complex, non-planar part geometries, a reinforcement shear-stress component must also be added to the component of the normal-stress while computing the overall compaction response of the fibrous reinforcement whenever the upper mould is dynamic. Although shear effects can be ignored for parts with shallow surfaces, they become significant for parts with steep surfaces [82]. A simple approach for finding the shear-stress is to first experimentally measure the coefficient of friction ($\mu_f$) between the fibrous reinforcement and the inner mould surface, as has been explained in [82]. The friction coefficient can then be used to compute the shear-stress according to,

$$\sigma_{shear} = \begin{cases} 0 & \text{if } \theta = 0 \\ \mu_f \sigma_f & \text{if } \theta > 0 \end{cases}$$  \hspace{1cm} (4.1)

Here $\theta$ is the acute angle between the local outward normal to the part surface and the direction of closure of the dynamic mould. $\sigma$ is the compaction-stress obtained
through the mixed-elastic model, and is a function of the fibre volume fraction. Following from Eq. (4.1), the total vertical force exerted on a dynamic mould by the fluid and fibres contained within a single element $\Omega_\text{e}$ of the flow mesh can be computed as,

$$p_{\text{clamp}}^{\Omega_\text{e}} = \begin{cases} \Delta (\sigma \cos \theta + \sigma_{\text{shear}} \sin \theta + p_{\text{avg}} \cos \theta) & \text{if } \frac{\partial h}{\partial c} \neq 0 \\ \Delta (\sigma \cos \theta + p_{\text{avg}} \cos \theta) & \text{if } \frac{\partial h}{\partial c} = 0 \end{cases} \quad (4.2)$$

where $p_{\text{avg}}$ is the average fluid pressure within the element. Note that when the mould is static, since there is no tendency of relative motion between the reinforcement and the mould, frictional forces are absent and therefore $\sigma_{\text{shear}}$ is dropped from Eq. (4.2).

4.1.1 Mixed-elastic model

In the mixed-elastic model, the behaviour of a single material is described using four nonlinear stress-volume fraction curves – one for when the material is dry and has thickness changing (“Dynamic Dry”), one when it is wet and has thickness changing (“Dynamic Wet”), one when it is dry and has static thickness (“Static Dry”) and a final one for when it is wet and has static thickness (“Static Wet”). A fourth-order polynomial, Eq. (4.3), provides excellent fit to the experimental data [1] for a wide range of fibre volume fractions and may subsequently be implemented for the force simulations.

$$\sigma(V_f) = a'V_f^4 + b'V_f^3 + c'V_f^2 + d'V_f + e'.$$  \quad (4.3)

where $a'$, $b'$, $c'$ and $d'$ are experimentally determined constants for the particular material in use. The details of the experimental material characterization procedure can be found in [1]. The values of the material constants for a glass-fibre chopped strand mat (CSM) are provided in Table 4.1. This material has an unloaded fibre volume fraction of approximately 20% and shall be considered for all computational experiments throughout the thesis. Note that the friction coefficient provided with Table 4.1 assumes sliding between a dry reinforcement and an aluminium mould [82].
Table 4.1: Mixed-elastic compaction model parameters for CSM [1], response in Pascal; valid for $25% \leq V_f \leq 50%$; $\mu_f = 0.185$ [82].

<table>
<thead>
<tr>
<th></th>
<th>Dynamic dry</th>
<th>Dynamic wet</th>
<th>Static dry</th>
<th>Static wet</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a'$</td>
<td>4.68e+7</td>
<td>2.96e+7</td>
<td>2.97e+7</td>
<td>4.55e+7</td>
</tr>
<tr>
<td>$b'$</td>
<td>-5.14e+7</td>
<td>-2.65e+7</td>
<td>-3.60e+7</td>
<td>-5.80e+7</td>
</tr>
<tr>
<td>$c'$</td>
<td>2.27e+7</td>
<td>9.50e+6</td>
<td>1.72e+7</td>
<td>2.84e+7</td>
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<tr>
<td>$d'$</td>
<td>-4.62e+6</td>
<td>-1.54e+6</td>
<td>-3.68e+6</td>
<td>-6.17e+6</td>
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<tr>
<td>$e'$</td>
<td>3.58e+5</td>
<td>9.03e+4</td>
<td>2.943e+5</td>
<td>4.95e+5</td>
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4.2 Simulation of Non-isothermal Rigid Tool LCM Processes

The procedure presented heretofore for non-isothermal resin flow simulations with clamping force predicting capabilities has been implemented through a Python code and shall be used in this section to simulate the effect of varying mould and resin temperatures on clamping force requirements. The simulations are carried out for two geometries; (1) a planar circular part and (2) a non-planar hemispherical part. Both parts are assumed to be injected with a reactive Ciba-Geigy epoxy resin system (Araldite LY 564 and Hardener HY 2954) [44], and contain the CSM as the reinforcing material. Properties of the resin are listed in Table 4.2 [44]; the essential thermal properties of glass-fibres are taken from Table 3.2 (in Chapter 3). The permeability $K$ of the isotropic CSM is expressed using the following exponential relation [2],

$$K = 3.07 \times 10^{-8}e^{-12.97V_f} \text{ (m}^2\text{).}$$  \hspace{1cm} (4.4)

Parameter combinations for the various simulation scenarios are detailed in Table 4.3. Both geometries consider the same parameter settings. Furthermore, both have a diameter of 1 m, are centrally injected through a 2 cm hole, and are considered to have a final cavity thickness of 7.5 mm. The dimensions are so chosen in order to detect possible geometry-induced variations in the vertical clamping force requirement, even when the planar projections of both geometries are exactly the same. Moreover, the large part dimensions allow the effects of spatial variations in the temperature and the degree of cure to be suitably magnified. The cavity thickness prior to the onset of dry fibre compaction, i.e. at $t = 0$, is assumed to be 10.5 mm (for the hemispherical part this corresponds to the maximum cavity thickness which occurs at the apex of the hemisphere) and the dry compression
speed is assumed to be 5 mm/min for all cases; these choices have little effect on subsequent force predictions.

Table 4.2: Epoxy resin properties [44].

<table>
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<tr>
<th>Physical and thermal properties</th>
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<tr>
<td>( \rho_r )</td>
<td>1087 kg/m(^3)</td>
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<tr>
<td>( k_r )</td>
<td>0.168 W/m K</td>
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<tr>
<td>( C_{pr} )</td>
<td>1260 J/kg K</td>
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<table>
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<tr>
<td>( A_1 )</td>
<td>0.5963 s(^{-1})</td>
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<tr>
<td>( A_2 )</td>
<td>57526.44 s(^{-1})</td>
</tr>
<tr>
<td>( E_1 )</td>
<td>21514.78 J/mol</td>
</tr>
<tr>
<td>( E_2 )</td>
<td>49435.55 J/mol</td>
</tr>
<tr>
<td>( m_1 )</td>
<td>0.5874</td>
</tr>
<tr>
<td>( m_2 )</td>
<td>3.2</td>
</tr>
<tr>
<td>( H_r )</td>
<td>4.641 ( \times ) 10(^8) J/m(^3)</td>
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<td>( \mu_0 )</td>
<td>5.787 ( \times ) 10(^{-11}) Pa s</td>
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<tr>
<td>( E_\mu )</td>
<td>56492 J/mol</td>
</tr>
<tr>
<td>( a_0 )</td>
<td>0.63</td>
</tr>
<tr>
<td>( a )</td>
<td>0.4202</td>
</tr>
<tr>
<td>( b )</td>
<td>0.00055(T – 298)(^2)</td>
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</table>

Table 4.3: Plan of simulations.

<table>
<thead>
<tr>
<th>Process</th>
<th>Final ( V_f )</th>
<th>( h_1 ) (cm)</th>
<th>( h_1 ) (mm/min)</th>
<th>( h_2 ) (cm)</th>
<th>( P_{inj} ) (kPa)</th>
<th>( T_m ) (K)</th>
<th>( T_r ) (K)</th>
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</thead>
<tbody>
<tr>
<td>RTM 1</td>
<td>0.35 0.5</td>
<td>0.75</td>
<td>0</td>
<td>0.75</td>
<td>400</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>RTM 2</td>
<td>0.35 0.5</td>
<td>0.75</td>
<td>0</td>
<td>0.75</td>
<td>400</td>
<td>330</td>
<td>300</td>
</tr>
<tr>
<td>RTM 3</td>
<td>0.35 0.5</td>
<td>0.75</td>
<td>0</td>
<td>0.75</td>
<td>400</td>
<td>330</td>
<td>330</td>
</tr>
<tr>
<td>RTM 4</td>
<td>0.35 0.5</td>
<td>0.75</td>
<td>0</td>
<td>0.75</td>
<td>400</td>
<td>330</td>
<td>350</td>
</tr>
<tr>
<td>CRTM 1</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
<td>200</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 2</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
<td>400</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 3</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
<td>200</td>
<td>330</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 4</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
<td>400</td>
<td>330</td>
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<tr>
<td>CRTM 5</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
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<td>330</td>
<td>350</td>
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<tr>
<td>CRTM 6</td>
<td>0.35 0.5</td>
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<td>1</td>
<td>0.75</td>
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<td>330</td>
<td>350</td>
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<td>CRTM 7</td>
<td>0.35 0.5</td>
<td>0.95</td>
<td>1</td>
<td>0.75</td>
<td>200</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 8</td>
<td>0.35 0.5</td>
<td>0.85</td>
<td>2</td>
<td>0.75</td>
<td>300</td>
<td>300</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 9</td>
<td>0.35 0.5</td>
<td>0.85</td>
<td>2</td>
<td>0.75</td>
<td>300</td>
<td>330</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 10</td>
<td>0.35 0.5</td>
<td>0.85</td>
<td>2</td>
<td>0.75</td>
<td>300</td>
<td>330</td>
<td>300</td>
</tr>
<tr>
<td>CRTM 11</td>
<td>0.35 0.5</td>
<td>0.85</td>
<td>2</td>
<td>0.75</td>
<td>300</td>
<td>330</td>
<td>330</td>
</tr>
<tr>
<td>CRTM 12</td>
<td>0.35 0.5</td>
<td>0.85</td>
<td>2</td>
<td>0.75</td>
<td>300</td>
<td>330</td>
<td>350</td>
</tr>
</tbody>
</table>

(\( h_1 \) = resin injection height; \( h_2 \) = secondary compression speed; \( h_2 \) = final cavity thickness; \( P_{inj} \) = resin injection pressure; \( T_m \) = mould temperature; \( T_r \) = resin injection temperature)
4.2.1 Planar-part simulation

Results are presented for the planar part first.

4.2.1.1 RTM process simulation

Figure 4.1: Effect of temperature variation on the force evolution and radial fluid pressure distribution for all RTM planar-part simulations (a) force evolution, (c) fluid pressure distribution for $V_f = 0.35$; (b) force evolution, (d) fluid pressure distribution for $V_f = 0.5$.

Figure 4.1 highlights the effect of varying the temperatures of the mould and the resin during RTM processes. The drop in resin viscosity with increase in temperature is seen to have the intuitive consequence of reducing the fill time. However, the temperature setting is seen to have a rather non-intuitive effect on the clamping force requirements. The force does not simply reduce with an increase in temperature, and the consequent drop in viscosity. The temperature difference between the mould and the resin plays a crucial role during resin injection for minimizing force requirements. It can be inferred from the Figures 4.1a and b that a high temperature difference between the mould and the resin, with the mould being
warmer than the resin, is essential in order to lower the clamping force. This can be explained by the radial variation in resin viscosity, resulting from the temperature distribution, which leads to a radial fluid pressure distribution as depicted in Figures 4.1c and d. In RTM 2, where the mould is significantly warmer than the resin, the fluid pressure is seen to be lower at all points within the mould. It is also interesting to note that heating the resin to a higher temperature than the mould causes the clamping forces during resin injection to be significantly higher than an ordinary isothermal process; as can be seen by comparing simulations of RTM 1 and 4. For the high fibre-volume fraction cases ($V_f = 50\%$) Figure 4.1b shows that the maximum force is in fact reached during the dry compaction phase.

4.2.1.2 CRTM process simulation

Reasonably low secondary compression speeds have been considered for the CRTM cycle in order to investigate the transition phase between the RTM and the CRTM processes. Applying high compression speeds would undoubtedly lead to significantly shorter fill times, but the corresponding clamping loads are often too high to be practical.

Prior to presenting the results it is important to describe the interpretation of the force evolution curve for CRTM processes. The force first peaks during the resin injection phase, which follows the dry compression of the fibrous reinforcement to the injection height. Once the required volume of resin has been injected the injection gate is closed, thereby causing the fluid pressure along with the total clamping force to fall. Post the injection phase the wet fibres are compressed at a constant velocity, causing the clamping force to rise once again due to the increase in fibre stress and fluid pressure.

Figure 4.2 shows the coupled effect of varying the resin injection pressure and the temperature conditions on the evolution of clamping force requirements, while keeping the resin injection height constant (CRTM 1-6). Unsurprisingly, processes with a higher injection pressure (CRTM 2, 4, 6) have shorter fill times but require larger clamping forces during resin injection. Moreover, the effect of the temperature elevation on the secondary compression phase of the cycle is also predictable. On comparing the elevated temperature simulations (CRTM 3-6) to
those with a lower temperature (CRTM 1 and 2), it is clear that the drop in resin viscosity does indeed lower the clamping force requirements during this phase. It can also be observed that although in 5 of the 6 cases the maximum force is reached during the wet compaction phase, in case of CRTM 6(a), the coupled effect of the high injection pressure and the resin being preheated to a temperature higher than that of the mould causes the force to peak during the resin injection phase instead.

Figure 4.3 depicts the coupled effect of the resin injection height and the temperature variations, while keeping the resin injection pressure constant (CRTM 7-12). Clearly, for a greater injection height (CRTM 7, 9, 11), the increased reinforcement porosity allows the resin to flow through with little obstruction, thereby leading to shorter resin injection times. As a flipside, the duration of the secondary compression phase is obviously longer for a fixed compression speed. Such a situation makes the design of an optimized manufacturing cycle non-trivial, since one cannot be sure whether the total resin fill time will be shorter or longer. For example, in the case of CRTM 7-10(a), using a higher resin injection height is seen to be more efficient in terms of filling time. However, for the case of CRTM 11(a) this behaviour is reversed.

On the other hand, for all the high fibre volume fraction scenarios, i.e. CRTM 7-12(b), using a higher injection height is seen to be consistently more efficient. Note however that this may not necessarily be the case when significantly higher resin injection pressures (above 1000 kPa) are employed.
Figure 4.2: Effect of resin injection pressure and temperature variation on the force evolution curves for planar-part CRTM simulations 1-6: (a), (c), (e) $V_f = 0.35$; (b), (d), (f) $V_f = 0.5$. 
Figure 4.3: Effect of resin injection height and temperature variation on the force evolution curves for planar-part CRTM simulations 7-12: (a), (c), (e) $V_f = 0.35$; (b), (d), (f) $V_f = 0.5$. 
4.2.2 Non-planar part simulation

Simulations for the hemispherical part are presented and analysed for geometry and shear stress induced variations in the force evolution curves.

4.2.2.1 RTM process simulation

Figure 4.4: Effect of temperature variation on the force evolution curve for all RTM non-planar part simulations (a) $V_f = 0.35$; (b) $V_f = 0.5$.

The trends seen in Figure 4.4 for the hemispherical part, in terms of the effects of temperature variation, are more-or-less the same as those observed for the case of the planar geometry. However, despite the two geometries having the same planar projection, the vertical clamping force requirements for the hemisphere are seen to be significantly greater. This happens primarily due to the resin pressure distribution, as the vertical component of the fibre response would be the same for both the cases (note that shear effects are absent during an RTM cycle). Additionally, the fill times for the hemispherical part are also significantly longer. This feature can be explained by the fact that the resin must traverse a longer, curved path before reaching the periphery of the part. The longer fill time also implies a higher degree of resin cure attained during filling. The resultant decrease in fluidity further adds to the time required by the resin to flow through the fibrous reinforcement and fill the part.
4.2.2.2 CRTM process simulation

Figures 4.5 and 4.6 show the effect of varying the resin injection pressure and the resin injection height, respectively, when applied to the non-planar part. These variations are made together with different mould and resin temperature combinations. The inferences drawn from these figures are very similar to those that were drawn for the circular part. This includes the importance of maintaining a high temperature difference between a warm mould and a colder resin in order to keep clamping forces low during resin injection. The only significant changes seen for the non-planar part are the considerably larger clamping force requirements during both the resin injection and the secondary compression phases, and the longer fill times. These are caused by, among other factors, the fibre volume fraction variations (and implicitly the in-plane permeability variations) in different areas over the surface of the hemisphere, and shear effects during mould compression.

4.2.3 Discussion

The results shown in this chapter indicate that an increase in temperature of the mould and/or the resin always leads to shorter fill times (resin degradation and/or resin gelation determine the theoretical upper limit of the applied temperature). Additionally, it is important to have a temperature differential between a heated mould and a colder resin in order to keep clamping forces low during resin injection. In case the forces peak during the resin injection phase, having a suitable temperature differential plays a vital role in minimizing setup costs. Moreover, the injection pressure, which directly affects the resin injection phase of the process, must be chosen such that a favourable balance between the fill time and the maximum tooling force is achieved. The resin injection height has a significant influence on both the injection phase as well as the wet compaction phase of the process. The choice of this height, along with the speed of secondary mould compression, is also critical in designing an efficient manufacturing cycle. These inferences lead to the belief that finding an optimal combination of process variables which allows a fast production cycle and an affordable setup is not a trivial task and requires a multicriteria optimization problem to be solved.
Figure 4.5: Effect of resin injection pressure and temperature variation on the force evolution curves for non-planar part CRTM simulations 1-6: (a), (c), (e) \( V_f = 0.35 \); (b), (d), (f) \( V_f = 0.5 \).
Figure 4.6: Effect of resin injection height and temperature variation on the force evolution curves for non-planar part CRTM simulations 7-12: (a), (c), (e) $V_f = 0.35$; (b), (d), (f) $V_f = 0.5$. 

(a) CRTM 7(a) - CRTM 8(a)
(b) CRTM 7(b) - CRTM 8(b)
(c) CRTM 9(a) - CRTM 10(a)
(d) CRTM 9(b) - CRTM 10(b)
(e) CRTM 11(a) - CRTM 12(a)
(f) CRTM 11(b) - CRTM 12(b)
4.3 Summary

In this chapter a mixed-elastic fibre compaction model has been used to capture the stress-strain behaviour of fibrous reinforcements. The model has been incorporated within a Python based fill simulation code in order to simulate the effect of temperature elevation on clamping force requirements during rigid-tool LCM processes. The friction occurring between the fibres and the mould wall during the dynamic mould phases has also been accounted for while computing the total internal force acting on the mould walls.

Analyses of the results presented for a circular and a hemispherical part indicate complex interactions between the various process variables, particularly during non-isothermal processes. In order to design an efficient manufacturing cycle these interactions need to be captured accurately. The non-intuitive nature of the effect of mould and resin temperature variations on the total internal forces, particularly during the resin injection phase, cannot be predicted easily without a simulation tool of the kind described in Chapters 2 and 3. The results, thereby, highlight the importance of the FE simulation package towards the ultimate goal of complete composites manufacturing cycle optimization.
Part 2

 Chapters 5 and 6

 Optimization
Chapter 5

Bilevel Multiobjective Optimization of LCM Processes

In this chapter the set of objectives considered in this research for optimizing the complete composites manufacturing cycle are first specified, followed by their evaluation procedure. A detailed mathematical description of the bilevel multiobjective optimization problem, which resembles a static Stackelberg game with multiple payoff functions for each player, is presented. It is shown that with certain adjustments made to the distribution of the design variables over the two critical phases of the manufacturing cycle, the problem under consideration can be made to fit into the bilevel framework. Moreover, modifications are introduced to an optimistic solution approach, discussed in previous studies [83, 84] and also in Section 5.4, in order to confine the search over more relevant areas of the design space. Having formulated the game-theoretic approach, a Bilevel Multiobjective Genetic Algorithm (BMOGA) is constructed for its implementation. The BMOGA is based on the popular multicriteria optimization routine – the elitist Nondominated Sorting Genetic Algorithm (NSGA-II), which is also briefly discussed.

5.1 Considered Design Objectives

A summary of the manufacturing problem structure is depicted in Figure 5.1, with the design objectives considered in this study contained within the bold solid blocks. Each objective is to be minimized. Minimization of the peak clamping force leads to a reduction in the equipment setup and running costs. Minimization of the manufacturing cycle time allows the output over any time-period to be maximized. Finally, the magnitude of the through-thickness temperature gradient during the curing phase of the process provides a simple heuristic measure of the magnitude of process induced residual stresses generated within the composite part, with the two quantities being directly related [47]. Therefore, the minimization of through-thickness temperature gradients ensures that the residual stresses are also kept down to a minimum, thereby maximizing the final part quality. Some additional criteria, specified in [47], can also be used as further measures of final part quality.
It should be noted that the optimization approach presented in subsequent sections is by no means restricted to handling only those design variables and objectives described above. Indeed, the framework is flexible enough to include many more. For example, the placement of resin injection gates and vents can be considered as additional design variables. Moreover, the minimization of dry areas within the mould during filling and the minimization of the total energy consumption over the entire manufacturing cycle are further objectives of interest that can be added in a straightforward manner to the ones already considered.

5.2 Objective Evaluation Procedure

The two levels of the bilevel framework shall be referred to as the upper level and the lower level. The filling phase of the process, which forms the lower level, is modelled using the hybrid FE/FD methodology described in Part 1 of this thesis. Although the FE/FD scheme is computationally much less demanding than a complete 3-D FE methodology, it is still too expensive to be incorporated into a population-based search strategy like a bilevel genetic algorithm. For this reason an Artificial Neural Network (ANN) based surrogate model, the choice and
construction of which shall be described in Chapter 6, is utilised for the lower level objective function evaluations.

The simulation of the cure phase, which forms the upper level, is on the other hand computationally inexpensive, and is directly integrated with the BMOGA for upper level function evaluations. For further cost reduction the simulation is carried out only at randomly chosen, yet well distributed reference points, over the part geometry. This is a valid simplification as in-plane heat conduction may be assumed to be negligible for parts of up to moderate thickness [70]. The simulation involves solving Eqs. (3.7) and (3.10) (without the convection terms) using the Crank Nicolson method and the fourth order accurate Runge-Kutta method, respectively, as discussed in Section 3.3. Ordinarily, the initial conditions required for simulating the cure phase, i.e. the temperature and cure distributions within the part at the end of filling, would be obtained through the fill simulation. However, the BMOGA does not explicitly use any numerical scheme that actually solves the flow/energy/chemical-species equations. Therefore, the temperature and cure distributions are also predicted through a trained ANN.

5.3 Multicriteria Optimization

A general multicriteria minimization problem is one which attempts to find all solutions \( x \in X \) such that the vector-valued mapping of the solution into the objective space, given by \( f(x) = (f_1(x), f_2(x), \ldots, f_m(x)) \), is minimized. Here \( X \subset \mathbb{R}^n \) is the set of all feasible points in the \( n \) dimensional design variable space, and \( m \) is the number of individual objectives to be minimized.

Consider two solutions \( x_1 \) and \( x_2 \), with \( x_1, x_2 \in X \). Then \( x_1 \) is said to dominate \( x_2 \) if and only if,

\[
\forall i \in \{1, 2, \ldots, m\}: f_i(x_1) \leq f_i(x_2) \text{ and } \exists j \in \{1, 2, \ldots, m\}: f_j(x_1) < f_j(x_2). \quad (5.1)
\]

A solution \( x_0 \) is said to be Pareto efficient or Pareto optimal if \( x_0 \in X \) and there exists no other feasible point \( x \) such that \( f(x) \) dominates \( f(x_0) \). Moreover, the images of the Pareto efficient solutions in the objective space constitute the Pareto front or Pareto surface.
From the definition of Pareto efficiency it is clear that for an \( m (> 1) \) dimensional objective space, the corresponding design variable space will generally have a set of Pareto efficient solutions instead of a single optimal solution. As has been stated in the introduction, this set includes every optimal solution of a reduced single objective problem with strictly positive objective weight combinations.

### 5.4 Bilevel Multiobjective Optimization

It is common practice in the LCM process optimization literature to convert the multicriteria optimization problem into a single objective by using a weighted sum of the normalized objective functions [47-49]. However, this approach demands prior knowledge of the form of the objective functions and the exact preferences of the decision maker (DM). Since such prior knowledge is generally not available, a multicriteria approach is used in this study. The mathematical description of a bilevel multiobjective minimization problem is as follows [64],

\[
\begin{align*}
\text{Minimize } & F(x_u, x_l), \\
\text{subject to } & x_l \in \arg\min \{ f(x_i) \mid g(x_i) \geq 0, h(x_i) = 0 \}, \\
& G(x_u, x_l) \geq 0, H(x_u, x_l) = 0, \\
& x_u = (x_1, \ldots, x_r); \ x_l = (x_{r+1}, \ldots, x_n), \\
& x_{l(i)} \leq x_i \leq x_{u(i)}, \ i = 1, \ldots, n.
\end{align*}
\]

In the description, \( F \) and \( f \) are the objective function vectors of the upper and lower level problem. \( G \), \( H \) and \( g \), \( h \) are, respectively, the upper and lower level constraints. \( x_u \) and \( x_l \) are the upper and lower level design vectors that together form \( x = (x_u, x_l) \), which is the \( n \) dimensional design vector of the overall problem. It is important to note that the lower level problem is optimized with respect to \( x_l \) only, while \( x_u \) acts as a fixed parameter. Therefore \( x_l \) can be considered to be a function of \( x_u \).

This formulation of the problem corresponds to an optimistic approach [83] wherein it is assumed that the DM controlling the lower level problem chooses, among all Pareto efficient solutions, the one which is best for the upper level. It can be argued that in general, and indeed for the composite manufacturing problem, this approach is overly optimistic. Several points on the Pareto front of the lower level problem may be totally irrelevant for the lower level DM. For example, in case of the composites manufacturing problem, minimization of the clamping forces and
the mould fill time are considered as the lower level objectives. It is possible to have a design which allows very low fill times but at the cost of unrealistically large clamping forces, or vice versa. However, such a configuration is unlikely to be ever chosen by the manufacturer. Furthermore, for points located close to the extremities of a convex Pareto front, it is always possible to make the marginal improvement in one objective significantly large when compared to the marginal worsening of some other objective. Therefore, such Pareto efficient solutions are generally considered less desirable. These arguments indicate that it would be incorrect to include all Pareto efficient solutions as equally desirable lower level solutions for the upper level problem. In order to tackle this issue a subdued-optimistic approach is taken by introducing the following modification to the mathematical description,

\[ x_i \in \{\text{argmin} \{f(x_i) \mid g(x_i) \geq 0, h(x_i) = 0\} \cap \{x_i: f(x_i) \in RI\}\} \tag{5.3} \]

where \( RI \) represents a region of interest in the objective space of the lower level DM. Therefore only those Pareto efficient solutions whose objective values lie within the region of interest are considered feasible for the upper level problem. Although it is difficult to make an a priori prediction of the region of interest, in [85] it was noted that “from practical experience... the user or designer usually picks a point in the middle of the surface...where the Pareto surface bulges out the most”. For a “convex bulge” of the Pareto front, it was defined to be the point below and farthest from the convex hull defined by the individual function minima. This point, also designated as the “knee”, is assumed to be the centre of the region of interest, the extent of which is predefined. It should be noted that selecting the solution in design variable space which maps to the knee as a unique solution of the lower level problem is also a viable option; however it may be too restrictive for the upper level DM. Selecting a set of equally desirable solutions within a preferred region lends greater robustness to the final approximation of the Pareto set obtained at the upper level.

5.4.1 Adaptation of the LCM process optimization problem

Returning to Figure 5.1, it is clearly possible for the filling phase to be optimized without taking the cure phase into account (as discussed in the introduction, this may lead to undesirable conditions during the cure phase). On the other hand, the
optimization of the cure phase must take into account the temperature and cure
distributions within the part at the end of filling. In order to fit the composites
manufacturing problem into the game-theoretic framework it is important to
redistribute the design variables amongst the DMs such that the objectives of the fill
phase may be affected by the design choices of the upper level DM (the one
controlling the cure phase). To this end, it is considered that the mould temperature
profile for the entire process, including the filling phase, is controlled by the upper
level DM. Note that it is also possible to transfer control of the injection
temperature of the resin to the upper level DM instead. However, complete process
temperature control should not be transferred, as in many cases this would allow
the cure phase to be optimized without taking the fill phase into account. As a result
of the redistribution of design variables, the mould temperature profile may be
viewed as $x_u$ while all other design variables constitute $x_l$. The objectives of the
lower level DM are to minimize the fill time and the clamping force requirements,
whereas the upper level DM attempts to minimize the cycle time (fill time + cure
time) and reduce residual stresses by minimizing the through-thickness
temperature gradients within the part during processing. In the present study the
gradient is approximated by the absolute value of the difference in temperature
between the surface and the core of the part (the temperature difference is
recorded only at each of the reference points at which the cure simulation is carried
out).

5.5 The NSGA-II Algorithm

The basic idea behind a genetic algorithm is to mimic natural evolution through
the Darwinian principle of survival of the fittest. The algorithm starts by randomly
generating a population of solutions. Each solution candidate is called an individual
and each iteration loop of the algorithm is called a generation. Over each generation,
“fit” solutions are selected as parent solutions that crossover or mutate to give rise
to a population of “fitter” offspring solutions. By increasing the fitness value over
subsequent generations, the genetic algorithm attempts to evolve into a more-or-
less static state, with a population that represents a good approximation to the true
Pareto efficient set. This derivative free approach has developed into a valuable tool
for global optimization in various applications wherein an analytical expression for
the objective functions is not available.

The following algorithm summarises the different steps involved in NSGA-II. The critical steps shall then be described in further detail.

- **Step 1**: Randomly generate initial population of $N$ solutions and initialize generation count as 1.

- **Step 2**: Assign each individual two fitness values: 1) a *nondominated front (NF)* and 2) a *crowding distance (CD)*.

- **Step 3**: Create a pool of $N/2$ parent solutions through a *binary tournament selection* strategy.

- **Step 4**: Crossover or mutate the parent solutions to obtain $N$ offspring individuals.

- **Step 5**: Reassign fitness values to each of the $2N$ available individuals. These $2N$ individuals form an intermediate population.

- **Step 6**: Select the $N$ fittest individuals among the $2N$ by using the NFs and the CDs lexicographically. The selected $N$ individuals form the population of the next generation.

- **Step 7**: Increment generation count by 1.

- **Step 8**: Go back to Step 3 or stop if prescribed number of generations is reached.

### 5.5.1 Fast nondominated sorting algorithm

This algorithm for sorting the individuals into different NFs was described in [59]. For each individual $i \in \{1, 2, \ldots, \text{population size}\}$ two entities are computed: 1) domination count ($n_i$), the number of individuals which dominate it and 2) the set of individuals that it dominates ($S_i$).

All solutions with $n_i = 0$ are assigned to the first NF. Then, $\forall i$ with $n_i = 0$, $n_j := n_j - 1 \ \forall j \in S_i$. If in doing so the domination count $n_q$ for any individual $q$ becomes zero, then that individual is added to a separate list $Q$. The members of $Q$ then form the
second NF and are used to continue the above procedure. The process is continued until all fronts are identified.

5.5.1.1 Constraint handling

In the presence of constraints, the definition of domination must be further generalised while comparing any two solutions $x_1$ and $x_2$, with $x_1, x_2 \in X$. A solution $x_1$ is said to constraint dominate $x_2$ if any one of the following conditions holds [59]:

1. $x_1$ satisfies all constraints while $x_2$ does not.

2. Both $x_1$ and $x_2$ violate some constraint but $x_1$ has a lower overall constraint violation.

3. Both $x_1$ and $x_2$ satisfy all constraints and $x_1$ dominates $x_2$ according to Eq. (5.1).

5.5.2 Crowding distance measurement

A good approximation of the Pareto front must ensure that the constitutive points are “well distributed” over the entire front. Therefore, the solutions which map to sparsely represented regions of the objective space (in other words, those which have a higher CD) must be assigned a higher fitness value. Quantitatively, the CD of an individual is a measure of the average distance, in objective space, between immediately neighbouring individuals on either side of the considered individual, when the population is sorted in ascending or descending order with respect to each of the objectives [59]. Moreover, boundary solutions (those with minimum or maximum objective function values) are assigned an infinite value of CD.

5.5.3 Binary tournament selection

Two solutions are picked randomly from the original population and then the best one is selected by using the NFs and CDs lexicographically.

5.5.4 Crossover operator

A Simulated Binary Crossover (SBX) operator, proposed in [86], is used in this study. It simulates, within a real-coded genetic algorithm, the one-point crossover properties of a binary-coded genetic algorithm. Corresponding design variables of
two individuals, $j$ and $k$, randomly selected from the parent pool recombine through the SBX operator to give two new offspring individuals, $j'$ and $k'$. The definition of the SBX operator starts with the observation that the average values of the design variables of the two parent solutions must be preserved. This implies,

$$x_j + x_k = x_j' + x_k' .$$  \hfill (5.4)

Moreover, a spread factor, $\beta_i$, is defined for the $i^{th}$ component of the design space, which equals the ratio of the spread of the offspring points and their parent points;

$$\beta_i = \left| \frac{x_j^i - x_k^i}{x_j^i - x_k^i} \right| .$$  \hfill (5.5)

A probability density function is defined for $\beta_i$ and is given by,

$$P(\beta_i) = \begin{cases} 0.5(\eta + 1)\beta_i^\eta & \text{if } \beta_i \leq 1 \\ 0.5(\eta + 1)\frac{1}{\beta_i^{\eta+2}} & \text{otherwise.} \end{cases}$$  \hfill (5.6)

Here $\eta$ is a probability distribution index which determines the likeness between the offspring and the parents. A higher value of $\eta$ increases the likelihood of producing offspring solutions that are very similar to the parents. A random number, $r_i$, is generated between 0 and 1, following which the area under $P$ is equated to $r_i$ in order to find the corresponding $\beta_i$. This is achieved through the following prescription,

$$\beta_i = \begin{cases} \left( \frac{1}{2r_i} \right)^{\frac{1}{\eta+1}} & \text{if } r_i \leq 0.5 \\ \left( \frac{1}{2(1-r_i)} \right)^{\frac{1}{\eta+1}} & \text{otherwise.} \end{cases}$$  \hfill (5.7)

Having obtained $\beta_i$, $x_j^i$, and $x_k^i$, can be computed by simultaneously solving Eqs. (5.4) and (5.5).

\textbf{5.5.5 Mutation operator}

Whenever two parent individuals do not undergo crossover, the design variables of each parent are passed through a mutation operator to give two new individuals.
The randomness involved in a mutation preserves diversity of the solutions and avoids premature convergence to a local front. The polynomial mutation operator for real-coded genetic algorithms, proposed in [86], is used in this study. It can be described as follows,

\[ x_j^i = x_j^i + (x_U^i - x_L^i) \delta_i. \]  

(5.8)

Here \( \delta_i \) is a perturbation factor, \( x_U^i \) and \( x_L^i \) are the upper and lower bounds of the \( i^{th} \) design variable, respectively. The probability density function of \( \delta_i \) is given by,

\[ P(\delta_i) = 0.5(\eta + 1)(1 - |\delta_i|)^\eta. \]  

(5.9)

The above density function is valid only in the range \( \delta_i \in (-1, 1) \). \( \eta \) is again a distribution index which plays a similar role as it does for the SBX operator. A random number \( r_i \in (0, 1) \) is again generated and the area under \( P \) is equated to \( r_i \) to find \( \delta_i \),

\[ \delta_i = \begin{cases} 
(2r_i)^{\frac{1}{\eta+1}} - 1 & \text{if } r_i < 0.5 \\
1 - (2(1 - r_i))^{\frac{1}{\eta+1}} & \text{otherwise}.
\end{cases} \]  

(5.10)

Thereafter, \( x_j^i \) is computed through Eq. (5.8).

**5.5.6 Migrating nondominated solutions to the RI**

Only those nondominated solutions of the lower level problem whose objective values lie within the \( RI \) are considered feasible for the upper level DM. For a robust solution, it is therefore important to get a dense and well distributed set of points within the \( RI \). Several algorithms have been proposed in the literature for achieving such a distribution [87-89]. A new procedure has however been used in this research. It begins with running the standard NSGA-II routine to first obtain a rough approximation of the Pareto front of the lower level problem. Two important points are then identified: 1) the nadir point, which is located in objective space and is defined by the “worst” objective values of all the Pareto efficient solutions, and 2) the ideal point, which is also located in objective space but is defined by the “best” objective values of all the Pareto efficient solutions. These points are then used to
normalize the objective values of the nondominated solutions to lie between 0 and 1. The solution closest to the knee is found according to its definition provided in Section 5.4. This solution is used as a reference point around which an \( (m-1) \)-sphere, with radius \( \text{rad} \) governed by the extent of the \( R_I \), is defined. Following this, the NSGA-II routine is rerun with a modified definition of the crowding distance \( CD_{\text{mod}} \).

5.5.6.1 Modified crowding distance measurement

\[
CD_{\text{mod}} = \begin{cases} 
CD + \left( \frac{1}{\text{rad}} \right) & \text{if } s_i \leq \text{rad} \\
\frac{1}{s_i} & \text{if } s_i > \text{rad},
\end{cases} \tag{5.11}
\]

where \( s_i \) is the Euclidean distance, measured in the normalized objective space, between the solution and the knee.

5.6 The BMOGA

Figure 5.2 shows a diagrammatic summary of the steps involved in the proposed BMOGA. It is constructed by nesting one NSGA-II algorithm within another. The outer simulation corresponds to the cure phase (upper level problem) whereas the inner simulation corresponds to the filling phase (lower level problem).

![Figure 5.2: The proposed BMOGA procedure.](image)
The algorithm starts with the generation of a population of mould temperature profiles at the upper level. During every function evaluation at the upper level, the mould temperature profile is sent to the lower level NSGA-II. The mould temperature during filling is extracted from the profile and it acts as a constant parameter according to which the lower level design variables are optimized. Once convergence onto the lower level Pareto front is achieved, the knee is used as a reference point to migrate the Pareto efficient solutions such that they satisfy Eq. (5.3). These solutions are returned to the upper level. Therefore, a single mould temperature profile leads to a large subpopulation of solutions. Cure simulations are carried out on each member of every subpopulation, based on the initial conditions of temperature and cure prescribed by the lower level design variables, to obtain the upper level objective functions. Further, all subpopulations at the upper level are concatenated and the usual NSGA-II procedure is performed to assign each member of every subpopulation an NF and a CD, based on the upper level objectives only. A particular mould temperature profile is recognized by the lowest (best) NF among members of its subpopulation and the highest CD among solutions with the lowest rank (all solutions in the subpopulation with higher ranks are eliminated). Selection operations at the upper level are based on these values of recognition. Crossover and mutation operations are performed on selected temperature profiles to generate new populations of solutions which are evaluated by recalling the lower level NSGA-II simulation. This procedure is repeated for a prescribed number of generations during which a good approximation of the Pareto front is hopefully achieved.

5.7 Summary

In this Chapter the structure of the complete optimization problem was introduced along with the new game-theoretic approach that has been adopted to solve it. A bilevel mathematical program was defined for the case of multiple objectives at each level, and a new subdued-optimistic approach was suggested for its solution. The popular NSGA-II routine was described, together with an algorithm for concentrated search around a preferred point. This routine was then used in a nested manner to construct the BMOGA for simulating the game between the decision makers at the two levels.
It is restated here that although a rather limited number of design variables and objectives have been treated in this research, the framework is flexible enough to include many more. The placement of injection gates and vents can be included as further lower level design variables. The minimization of void content is an important criterion that can be included as another lower level objective, while total process energy consumption can form an additional upper level objective.
Chapter 6

Optimization Examples

This chapter first considers the manufacturing of a composite disc as an illustration of the optimization approach. During application of the BMOGA to this test case, the process of identifying the feasible region of the design variable space and the construction of a preferred surrogate model are explained. The parameter settings used to run the BMOGA are specified. The results obtained through the optimization algorithm, both at the upper and lower levels, are then analysed and discussed in some detail.

The procedure carried out for the case of a simple composite disc is then repeated for optimizing the manufacturing cycle of a complex industrial part. This latter task highlights the efficacy of the proposed game-theoretic approach when applied to a real world manufacturing problem.

6.1 Manufacturing a Composite Disc

The proposed framework is now applied for optimizing the production cycle of a circular composite part manufactured by the CRTM process. The diameter of the part is 1 m with a central injection hole of 2 cm. The thickness of the finished part is assumed to be 1.5 cm, which is moderately thick, and the final fibre volume fraction is approximately 35%. The thickness has been so chosen in order to encourage development of significant through thickness temperature gradients, as a test of the robustness of the optimization procedure. The glass-fibre CSM and the epoxy resin system considered in Chapter 4 are chosen to be the constituent materials (the parameters of the fibre compaction model and the material properties can be found in Tables 3.2, 4.1, 4.2).

6.1.1 Determining feasible bounds of the design space

Prior to building the surrogate model, the fill simulation code is used to carry out a preliminary study of the design space in order to determine the bounds of the design variables within which the resin is unlikely to cure prematurely, i.e. during
mould filling. Moreover, the resin velocity during filling should be kept low enough so as to prevent any significant deformation of the fibrous reinforcement (a phenomenon called fibre washing [54]) resulting from excessive viscous drag and/or form/pressure drag. The latter requirement places further constraints on the upper bound of the resin injection pressure, as well as that of the mould and resin temperatures. During the curing phase it should be ensured that the final dwelling temperature of the mould is high enough, i.e. close to the maximum glass transition temperature \( T_{g,\infty} \) of the resin, in order to allow the resin to cure sufficiently. Having a low curing temperature causes the resin to vitrify (transition from a liquid or rubbery state to a glassy state [90]) before it reaches an acceptable degree of cure. As the reduced molecular mobility caused by vitrification almost completely quenches the polymerization reaction [90, 91], the progress in the degree of resin conversion is essentially stalled. Consequently, the mechanical properties of the finished part remain underdeveloped. In addition to the mould temperature requirements, an upper bound is placed, in the form of a constraint, on the maximum exothermic temperature allowed anywhere within the part during the manufacturing cycle. Doing so prevents the selection of a combination of design variables which would cause degradation of the polymer matrix due to overheating.

<table>
<thead>
<tr>
<th>Lower level design variables ((x_l))</th>
<th>Description</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection pressure ((P_{\text{inj}}))</td>
<td>200 KPa</td>
<td>500 KPa</td>
<td></td>
</tr>
<tr>
<td>Injection height ((h_{\text{inj}}))</td>
<td>1.6 cm</td>
<td>2 cm</td>
<td></td>
</tr>
<tr>
<td>Secondary compression speed ((V_{\text{wet}}))</td>
<td>0.5 mm/min</td>
<td>2.5 mm/min</td>
<td></td>
</tr>
<tr>
<td>Resin temperature</td>
<td>293 K (20 °C)</td>
<td>348 K (75 °C)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Upper level design variables ((x_u))</th>
<th>Description</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mould temperature during filling</td>
<td>293 K (20 °C)</td>
<td>333 K (60 °C)</td>
<td></td>
</tr>
<tr>
<td>Mould heat rate</td>
<td>2 K/min</td>
<td>30 K/min</td>
<td></td>
</tr>
<tr>
<td>Final mould temperature</td>
<td>393 K (120 °C)</td>
<td>433 K (160 °C)</td>
<td></td>
</tr>
<tr>
<td>Maximum exothermic temperature allowed</td>
<td>500 K (227 °C)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The bounds of the design variables considered for the present test case have been set according to the factors mentioned above, and are specified in Table 6.1. Note that the process is assumed to begin with the mould walls separated by 2.1 cm and an initial dry compression speed of 5 mm/min. The lower bound of the
injection height is greater than the final part thickness to ensure that the process is CRTM. For simplicity only a single temperature ramp is considered during the cure phase. For complex resin systems a more intricate mould temperature profile, with multiple ramps and dwelling periods, can be applied [47, 48]. The subsequent increase in the number of design variables of the cure phase alone, which have no bearing on the progress of the fill phase, further reinforces the claim made here that a centralized approach, i.e. a single combined level of optimization, is inappropriate.

6.1.2 Building a dataset

Having determined the bounds of the lower level design variables and the mould temperature during filling, sample points within the feasible design space are selected for carrying out computer experiments. The data from these points are subsequently used to train the surrogate model. The selection of the points is based on a Latin Hypercube Sampling (LHS) technique, which ensures that the chosen design points are non-collapsing, i.e. there exist no two design points with even a single common parameter value [65]. As a result the points are more-or-less evenly distributed when projected along any parameter axis. Moreover, in order to ensure even distribution of the points throughout the design space, an optimized LHS technique is used, one which attempts to maximize the minimum Euclidean distance between any two points in the design space. The algorithm used for doing this is presented in [65]. Determining the number of sample points depends on a trade-off between the desired accuracy level and the computational resource consumption.

6.1.3 Surrogate modelling

Surrogate models are often used in conjunction with genetic algorithms when the objective functions are too computationally expensive [92]. These models learn to approximate the underlying function form describing a set of data, and can then be used to efficiently evaluate objective values for any point in the function domain. Popular surrogate modelling techniques include the response surface method, Kriging and ANNs. Of these, Kriging and ANNs have been used previously in an LCM process optimization setting [67, 93]. However, in [94] it was shown that, at least for the type of objectives being evaluated in this study, ANNs are superior in terms
of both prediction accuracy and computational efficiency. They have therefore been adopted as the preferred surrogate model for the test cases presented herein.

The most commonly used ANN is the simple feed-forward Multilayer Perceptron (MLP). Figure 6.1 shows an example of the MLP. The layers include an input layer, an output layer, and one or more hidden internal layers [95], the neurons (circular nodes) of which are interconnected by links which assign a weighting factor to the signals they carry. Deciding on the weights forms part of training the ANN and shall be discussed later.

![Figure 6.1: A simple Multilayer Perceptron.](image)

Although the MLP is widely used, there exist areas of concern which require special focus. Most important among them is the selection of the number of hidden layers and the number of neurons in each layer [95]. A lack of knowledge of the function behaviour or of the efficacy of the training algorithm often leads to either an inadequate number or too many hidden neurons to be specified. In order to overcome the difficulties associated with the MLP, the Cascade-Correlation Learning Architecture Neural Network (CCA-NN), first presented in [66], is employed in this study. The CCA-NN determines its own neural topology during the training procedure, thereby making it unnecessary to possess any prior knowledge of the objective function form or the underlying training algorithm.

### 6.1.3.1 The CCA-NN

During its learning process the CCA-NN adds one hidden neuron to the network
at a time through a learning algorithm which maximizes the magnitude of the correlation between the output \( V \) of the new neuron and the residual error \( E \) to be eliminated [66]. The neuron receives input signals from the external inputs as well as each of the existing hidden neurons in the network. The \( V \) to \( E \) correlation \( S \) is defined as [66],

\[
S = |\sum_p (V_p - \bar{V})(E_p - \bar{E})|. \tag{6.1}
\]

Here \( p \) represents the points selected from the feasible region of the design space. \( \bar{V} \) and \( \bar{E} \) are the mean values of \( V \) and \( E \), respectively, over all \( p \). The quickprop algorithm, described in [96], is used to assign the added neuron's incoming link weights, so as to maximize \( S \). Once these weights have been determined, they remain frozen through the entire training procedure. Post the addition of a new neuron, its output link weights, together with the weights of all existing output links, are recomputed so as to minimize the squared error at the output. This recomputation is again performed through the quickprop algorithm. If the total squared error is reduced to a prescribed limit the training is stopped, else another hidden neuron is added and the above procedure is repeated. Figure 6.2 summarizes the steps involved in constructing a CCA-NN.

In the present study for the manufacturing of a composite disc, 300 sample points are selected through the optimized LHS sampling technique and used to train the CCA-NN. As simple axisymmetric elements are used for this simulation, the total computational expenditure up to the building of the surrogate model is negligible. Moreover, the trained surrogate is found to make very good predictions even in unsampled regions of the design space. It is important to note that this number is significantly lower than the number of function evaluations required by even a single lower level NSGA-II call. The cross-validation results from the trained network are depicted in Figure 6.3. The correlation coefficient \( (R) \), appearing in Figure 6.3, is a measure of the strength of the linear relationship between the surrogate’s prediction and the output from the computer simulation. It is given by,

\[
R = \frac{\sum_{i=1}^{n}(X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2} \sqrt{\sum_{i=1}^{n}(Y_i - \bar{Y})^2}} \tag{6.2}
\]
Figure 6.2: Summary of the CCA-NN training procedure. The vertical lines indicate incoming signals. The boxed connections have frozen weights while the x connections are repeatedly trained [66].

Here $X_i$ is the output of the computer simulation at the $i^{th}$ sample point and $Y_i$ is the corresponding surrogate model prediction. $n$ is the total number of sample points used. From the Cauchy-Schwarz inequality it can easily be shown that the value of $R$ must lie between -1 and +1. The closer the surrogate model’s predictions to the computer simulation, the closer $R$ is to +1. Furthermore, the relative error plots in Figure 6.3 show that the majority of the CCA-NN force predictions are within a 5% error band. For the injection time predictions, the errors are slightly larger at small values of time, although the majority remains within a 10% error band.
Figure 6.3: Comparison of CCA-NN predictions against actual function evaluations.
6.1.4 Applying the BMOGA

The BMOGA is implemented on a MATLAB platform, and the MATLAB Parallel Computing Toolbox is utilized to parallelize computations for the upper level population on 4 cores of an Intel Core i5 CPU running at 3.33 GHz. While running the NSGA-II simulation the following parameter setting is used: crossover probability of 90%, mutation probability of 10%, distribution indices for the real-coded genetic operators are chosen to be 15 and 5 for the crossover and mutation operators, respectively. The lower level solutions are evolved using a population size of 40 individuals, initially over 60 generations to obtain a rough approximation of the complete Pareto front, and then for 30 further generations to focus the search within the $RI$. The radius of the $RI$ is set as 0.2 in the normalized objective space. For the upper level problem a population size of 30 individuals is considered, which is evolved over 75 generations. For the chosen population sizes and generation counts, the total runtime of the BMOGA is approximately 10 hours.

Figures 6.4a and 6.4b show the results in objective space obtained from the lower level NSGA-II, by considering the mould temperature to be a constant parameter. The figure depicts the evolution of the solutions over three steps: the image in objective space of the initially generated population, points converged onto the Pareto front, and finally, efficient points migrated within the region of interest around the knee. The final set of solutions is returned to the upper level NSGA-II.

Figures 6.5a and 6.5b show the force evolution curves for randomly chosen Pareto efficient solutions. The similarity between the peak forces reached during the injection and compression phases validate the Pareto efficiency of the solutions. This can be explained by the following example - keeping the peak force during one phase constant, the peak force during the other could be reduced using either lower injection pressure or wet compaction velocity, thereby leading to an inefficient solution in terms of fill time.

In this study the cure simulations at the upper level are continued until a minimum of 90% cure is reached at all the reference points. Figure 6.6 shows the Pareto front obtained after the complete bilevel optimization procedure. The figure
also depicts the image of the randomly chosen initial population in the upper level objective space. The initial population is seen to form several clusters, each corresponding to a lower level NSGA-II call. All of these clusters are far away from the final Pareto front, thus highlighting the importance of the optimality study. Having obtained the set of efficient solutions, the manufacturer can choose the most preferred one based on the application of the part. If a high quality part is needed, a solution with its image close to Minimum 1 must be chosen. On the other hand, if the quality of the part can be compromised, a solution that maps close to Minimum 2 should be chosen.

Figure 6.4: Results in objective space of the lower level problem, obtained through NSGA-II simulations for two different mould temperatures: (a) 300 K and (b) 330 K.

Figure 6.5: Force evolution curves for randomly chosen Pareto optimal solutions from Figures 6.4a and 6.4b.
Figure 6.6: Results in objective space of the upper level problem, obtained after a complete BMOGA simulation for the case of a composite disc.

Figures 6.7a-6.7f depict the force evolution and the mid-radius (0.25 m from the centre of the part) temperature and degree of cure evolution curves for the solutions representing the individual objective function minima of the upper level problem. Note that in Figure 6.7d the peak force reached during the resin injection phase is greater than that reached during the compression phase. However, this does not preclude Pareto efficiency as the wet compaction velocity for this case is equal to the supplied upper bound and cannot be increased further. In Figure 6.7b although the cure time is high, the temperatures at the surface and core of the part evolve uniformly, which minimizes residual stresses within the part. On the other hand, in Figure 6.7e, although the resin rapidly reaches the desired cure level, large temperature gradients are induced which may cause high residual stresses within the part. Uniformity in the surface and core temperatures generally implies uniformity in the evolution of the degree of cure as well, as depicted in Figure 6.7c. This is another factor that ensures the minimization of residual stresses [47, 48]. An important point to note here is that although large through thickness cure gradients are in general undesirable, a core to surface cure progression is more favourable than a surface to core one [55].
Figure 6.7: Force (a & d), temperature (b & e) and degree of cure (c & f) evolution curves of the solutions representing the individual function minima in Figure 6.6.
6.2 Manufacturing a Fireman’s Helmet

Next a complex curved, 3-D geometry of a fireman’s helmet is considered for testing the optimization approach. The part geometry has been obtained from Pacific Helmets Ltd, of Wanganui, New Zealand. It has a length of approximately 0.42 m, width of 0.32 m, and a depth of 0.17 m. Due to symmetry only one half of the geometry has been modelled. The mesh used is depicted in Figure 6.8. It consists of 475 vertices and 879 elements, which include obtuse triangles. Yet, sufficiently converged results are obtained with this mesh. The position of the resin injection gate has been pre-specified as this is not part of the design variables considered in the present study. However, as has been mentioned previously, the gate and vent locations can easily be included as additional design variables without any change to the overall optimization procedure.

The helmet has a uniform thickness of 2 mm throughout, which is rather thin, and the final fibre volume fraction of the glass-fibre CSM is approximately 40%. For the given dimensions, the volume to be filled by resin equates to $1.07255 \times 10^{-4} \text{ m}^3$. In
order to demonstrate the robustness of the fill simulation code when used for a complex geometry modelled with mixed, i.e. acute and obtuse, triangular elements, trial simulations were first carried out for RTM and CRTM processes. A simple isothermal filling of the mould was performed with a non-reactive resin of viscosity 0.25 Pa.s. The results are depicted in Figure 6.9. In particular, the constant injection rate RTM simulation depicted in Figure 6.9c, for which the theoretical fill time should be precisely 200 seconds, predicts it to be 201.34 seconds. The excellent agreement shows that the mass conservation errors induced by the existence of obtuse triangles in the FE mesh are insignificant.

Figure 6.9: Force evolution curves for isothermal filling simulations: (a) RTM cycle with constant pressure injection, (b) CRTM cycle with constant pressure injection and (c) RTM cycle with constant injection rate.
During the curing cycle of such thin parts, significant through-thickness temperature gradients are not expected to develop as the heat generated due to resin polymerization is rapidly conducted to the mould walls. The results of the optimization study shall be used to confirm this prediction. Although the product is currently manufactured by the RTM process, optimization is carried out for a CRTM production cycle. The bounds of the design variables are listed in Table 6.2. The initial mould separation is taken to be 4 mm, with a dry compression speed of 5 mm/min, for all cases. As the assumed material constituents are the same as the composite disc case (including the epoxy resin system), so are the design variable bounds, except of course for the resin injection height.

<table>
<thead>
<tr>
<th>Description</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection pressure ($P_{inj}$)</td>
<td>200 KPa</td>
<td>500 KPa</td>
</tr>
<tr>
<td>Injection height ($h_{inj}$)</td>
<td>2.5 mm</td>
<td>4 mm</td>
</tr>
<tr>
<td>Secondary compression speed ($V_{wet}$)</td>
<td>0.5 mm/min</td>
<td>2.5 mm/min</td>
</tr>
<tr>
<td>Resin temperature</td>
<td>293 K (20 °C)</td>
<td>348 K (75 °C)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Description</th>
<th>Lower bound</th>
<th>Upper bound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mould temperature during filling</td>
<td>293 K (20 °C)</td>
<td>333 K (60 °C)</td>
</tr>
<tr>
<td>Mould heat rate</td>
<td>2 K/min</td>
<td>30 K/min</td>
</tr>
<tr>
<td>Final mould temperature</td>
<td>393 K (120 °C)</td>
<td>433 K (160 °C)</td>
</tr>
<tr>
<td>Maximum exothermic temperature allowed</td>
<td>500 K (227 °C)</td>
<td></td>
</tr>
</tbody>
</table>

For the case of the fireman’s helmet the simulations at the 300 sample points add up to 26 hours of runtime. The comparison results of the built surrogate, as depicted in Figure 6.10, show that the surrogate model successfully learns the behaviour of the objective functions to a very high degree of precision. The trained CCA-NN is used to run lower level function evaluations of the BMOGA, the parameter settings of which are the same as the previous test case. The final result obtained at the upper level of the bilevel problem is depicted in Figure 6.11.
Figure 6.10: Comparison of CCA-NN predictions against actual function evaluations

(a) Computationally obtained injection times (seconds) vs. CCA-NN prediction (seconds)
- Obtained points
- Ideal fit
- $R = 0.999$

(b) Computationally obtained peak force during injection (N) vs. CCA-NN prediction (N)
- Obtained points
- Ideal fit
- $R = 0.999$

(c) Computationally obtained peak wet compression force (N) vs. CCA-NN prediction (N)
- Obtained points
- Ideal fit
- $R = 0.999$

(d) Absolute relative error (%) for injection times
- Obtained points
- Ideal fit

(e) Absolute relative error (%) for peak force during injection

(f) Absolute relative error (%) for peak wet compression force
Figure 6.11: Results in objective space of the upper level problem, obtained after a complete BMOGA simulation for the case of the fireman's helmet.

The slight difference in temperatures between the surface and the core of the helmet, for all points located on the Pareto front approximation, is in agreement with the prediction made for the curing cycle of thin parts. As a result, the temperature gradient induced residual stresses are unlikely to be significant. It is therefore advisable to select the solution that minimizes cycle time. The combination of design variables corresponding to this solution (i.e. Minimum 2 in Figure 6.11) is provided in Table 6.3. Moreover, complete simulations of the filling and curing phases are provided in Figure 6.12; the temperature and cure evolutions are for a randomly selected point within the part. It can be seen in Figure 6.12a that unlike for the case of the composite disc, the clamping force requirement peaks during the secondary compression phase, and indeed by a significant margin. It is therefore trivial to conclude that the resin injection pressure must be kept as high as possible; or at the upper bound, as is the case for Minimum 2. Moreover, since the excess heat generated within the part rapidly dissipates to the mould walls, one may consider allowing high temperature conditions in order to accelerate the filling and curing phases, without being too concerned about overheating within the part (see Figure 6.12b). This intuition too is found to be true for the case of Minimum 2.
However, the choice of the resin injection height and the secondary compression speed, which ensures the image of the solution to exist within the knee region of the Pareto front, remain non-trivial.

Table 6.3: Design variables corresponding to Minimum 2 in Figure 6.11.

<table>
<thead>
<tr>
<th>Lower level variables</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection pressure ($P_{inj}$)</td>
<td>500 KPa</td>
<td></td>
</tr>
<tr>
<td>Injection height ($h_{inj}$)</td>
<td>2.574 mm</td>
<td></td>
</tr>
<tr>
<td>Secondary compression speed ($V_{wet}$)</td>
<td>1.455 mm/min</td>
<td></td>
</tr>
<tr>
<td>Resin temperature</td>
<td>348 K (20 °C)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Upper level variables</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mould temperature during filling</td>
<td>333 K (20 °C)</td>
<td></td>
</tr>
<tr>
<td>Mould heat rate</td>
<td>30 K/min</td>
<td></td>
</tr>
<tr>
<td>Final mould temperature</td>
<td>433 K (120 °C)</td>
<td></td>
</tr>
</tbody>
</table>

Figure 6.12: Force (a), temperature (b) and cure (c) evolution curves for Minimum 2.
6.3 Summary

In this chapter the different steps involved in setting up the problem, prior to running the BMOGA, were discussed. These steps begin with the essential considerations for determining the feasible bounds of the design variable space, followed by the selection of well distributed sample points within that space and finally, building the artificial neural network based surrogate model from simulation data at those points. The bilevel optimization approach was then applied to two manufacturing test cases, (a) a moderately thick planar composite disc, and (b) a fireman’s helmet of low part thickness. For the case of thick parts it was found that having a fast cycle time was coupled with high through-thickness temperature/cure gradients during curing. Therefore, for high-end applications (e.g. the aerospace industry) a significant compromise might have to be made in terms of the production time in order to maximize part quality. On the other hand, for thin parts, the heat generated during resin cure gets rapidly conducted to the mould walls, thereby leading to uniformity of the temperature profile at the core and the surface of the part. This feature allows the manufacturer to have a faster cycle time as compared to that of a thick part manufactured with the same material constituents.

Overall, it was shown that modelling the optimization problem as a Stackelberg game provides solutions that are efficient with respect to the objectives of both the DMs. The solutions are not skewed in favour of the objectives of either the filling or the curing phase. Moreover, presenting the final result as a diverse set of Pareto efficient solutions allows the manufacturer to choose the most preferred solution \textit{a posteriori}, without the need to supply any prior weights to the objective functions.
Chapter 7

Conclusions, Achievements and Future Work

The objective of this research was twofold. It comprised of 1) finding a set of numerical procedures best suited for solving the coupled flow/energy/species equations occurring in non-isothermal, rigid-tool LCM processes, and 2) developing an optimization procedure capable of handling the filling and curing phases of these processes in a coupled manner, so as to allow fast and low cost production of high quality parts. In this concluding segment of the thesis, some of the key findings and solution methodologies proposed in this work, towards the specified objective, are compiled and presented. This is followed by research achievements in the form of publications in refereed journals and conference proceedings. Finally, some recommendations are made for further research which would help enlarge the domain of validity and improve the performance of the solution techniques proposed.

7.1 Conclusions

The major contributions of the different chapters in this thesis are as follows:

• Chapter 2 – The FE formulation to solve the fundamental resin flow equation was detailed in this chapter. It was rigorously shown that the chosen non-conforming elements ensured resin mass conservation for both the RTM and the CRTM cases. Moreover, a validation study of the developed FE code was carried out against analytical results, for the manufacture of a hemispherical part. The comparison results strongly verified the accuracy of the code.

• Chapter 3 – The governing flow equations were extended to include the case of non-isothermal mould filling with a reactive resin. The partial differential equation modelling this phenomenon is convective-diffusive, with a dominant first derivative. A previously proposed efficient hybrid FE/FD procedure was enhanced to deal with the dynamic mould phase of the CRTM process, in the limiting case of predominantly in-plane resin flow; note that this limiting case
actually forms the majority in composites manufacturing. Moreover, it was shown that the classical Galerkin FE scheme is inadequate to tackle the dominant convection term. A study of different stabilized variants of the scheme was undertaken, which led to the identification of a modified form of the nonlinear, discrete maximum principle satisfying Mizukami-Hughes Petrov-Galerkin (MHPG) scheme as being most accurate for the problem under consideration. The linear Streamline Upwind Petrov-Galerkin (SUPG) scheme was however found to be computationally most efficient. It was noted that the MHPG procedure had never previously been used in an LCM simulation setting.

- Chapter 4 – A Python based FE simulation code, enhanced with the ability to tackle cases with dynamic moulds and non-isothermal processing conditions, was developed and utilized to study, among other factors, the effect of temperature changes of the mould and the resin on the clamping force requirements and fill times of rigid-tool LCM processes. Not only did the simulations highlight the complex interactions between the various process variables in terms of their effects on force and time, but also revealed a rather non-intuitive relationship between the mould and resin temperatures, particularly during the resin injection phase. It was observed that allowing a high temperature difference between the mould and the resin, with the mould being warmer than the resin, lead to significant reductions in clamping force requirements. On the other hand, heating the resin to a higher temperature caused the clamping forces during injection to be higher than an ordinary isothermal process. Overall, the chapter showed the significance of the simulation package towards finding a process design with optimal trade-off between equipment setup and running costs, and the manufacturing time.

- Chapter 5 – The dual phase (filling and curing) manufacturing cycle was modelled as a two player static Stackelberg game, with multiple objectives for each player. The leader was assumed to control the curing phase while the follower controlled the filling phase. The design variables of the complete process were distributed between the players in a manner that neither could optimize their own phase independently of the other. Such an approach was taken as handling the phases independently in a sequential optimization
procedure could often lead to extremely limiting or completely unfit environments for the latter optimized phase. A subdued-optimistic variant of the more traditional optimistic approach to solving the multicriteria Stackelberg game was proposed in order to account for the fact that all Pareto efficient solutions are not necessarily equally desirable. This approach was implemented through a Bilevel Multiobjective Genetic Algorithm (BMOGA), which was constructed by nesting one NSGA-II algorithm within another; with the outer algorithm representing the leader’s problem and the inner one representing the follower’s problem.

- Chapter 6 – The developed BMOGA was applied to two test cases, for manufacturing 1) a flat composite disc, and 2) a fireman’s helmet, by the CRTM process. The different steps involved prior to running the BMOGA were described; i.e. 1) selecting a set of well distributed sample points in the design space, at which the simulation package is run to generate a dataset of the required objectives, and 2) building an artificial neural network based surrogate to the simulation code through the generated dataset. The results of the BMOGA were shown to be efficient with respect to the objectives of both players. Moreover, it is clear that, unlike previous approaches, obtaining the final optimization result in the form of a diverse set of Pareto efficient solutions allows the manufacturer to choose the most preferred one a posteriori. There is no need to make any prior decisions on the importance level (or weighting) of each of the different objectives. Additionally, the second test case showed the efficacy of the approach when applied to a complex real word manufacturing problem.
7.2 List of Publications

7.2.1 Refereed journals


7.2.2 Conference proceedings


7.3 Recommendations for Future Work

- The developed FE simulation code does not utilize the features of the solution procedure in terms of parallelizability. As has been mentioned in the thesis, the node-wise solution of the through-thickness heat conduction equation and the layer-wise procedure for the in-plane convection-diffusion equation provide a solution structure that can be parallelized in a rather straightforward manner. The increased speed through the use of multiple cores would allow high-fidelity simulations to be run. It should also be noted that the element-wise solution procedure of the DG method provides further scope for parallelization within each in-plane layer. This encourages further study into the application of advanced DG methods, which according to the enhancement introduced in Eq. (3.87) is the only one that explicitly handles the divergent velocity field during the dynamic mould phase.

- For non-isothermal simulations of predominantly in-plane flows, the MHPG scheme, with some modifications, has been shown to be the most accurate. However, the method is well described only for the case of 2-D triangular elements and does not have an immediate extension to 3-D. Further development of this method would allow high-fidelity simulations even for the comparatively rare case of thick part manufacturing, wherein through-thickness resin flow is appreciable.

- While solving the bilevel multiobjective optimization problem through the subdued-optimistic approach, the knee is assumed \textit{a priori} to be the reference point of interest. Although this seems to be a reasonable assumption, it is not necessarily the case always. Therefore, there exists the need for developing algorithms which can incorporate the preferences of the follower in a more flexible, and ideally interactive, manner. Although algorithms enabling progressive interaction with the leader are available [97], performing the same with the follower will be significantly more challenging.
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Appendix A

Mathematical Derivations and Further Results for Chapter 3

This appendix first presents the mathematical derivation of the result pertaining to the transformation of the modified Bessel differential equation, given in Chapter 3. In Section A.2 a through-thickness mesh refinement analysis is carried out to check the effect of progressively increasing the grid Fourier number on solution accuracy. Finally, the accuracy of an SUPG based non-isothermal filling simulation for a non-planar part is tested against analytically derived solutions.

A.1 Transformation of the Modified Bessel Differential Equation

The derivation provided is based on the transformation of the standard Bessel differential equation presented in [98].

Let,

\[ y = x^\eta I_m(\beta x), \]  

(A.1)

where \( I_m(x) \) is the modified Bessel function of the first kind, and,

\[ \eta = \frac{y}{x^\eta}, \xi = \beta x. \]  

(A.2)

Therefore, \( \eta \) and \( \xi \) satisfy the following second-order ordinary differential equation (also called the modified Bessel differential equation),

\[ \xi^2 \frac{d^2 \eta}{d\xi^2} + \xi \frac{d\eta}{d\xi} - \left( \xi^2 + m^2 \right) \eta = 0. \]  

(A.3)

Eq. (A.3) can be written as,

\[ \xi \frac{d}{d\xi} \left( \xi \frac{d\eta}{d\xi} \right) - (\xi^2 + m^2) \eta = 0. \]  

(A.4)

Since,
one has,

\[ \frac{\xi d\eta}{d\xi} = \frac{\xi d\eta}{d\xi} = x \frac{d\eta}{dx}. \quad (A.5) \]

Moreover,

\[ \frac{\xi}{d\xi} \left( \frac{\xi d\eta}{d\xi} \right) = x \frac{d}{dx} \left( x \frac{d\eta}{dx} \right). \quad (A.6) \]

Substituting Eqs. (A.2), (A.6) and (A.8) into Eq. (A.4) and simplifying, one has,

\[ y'' - \frac{(2y-1)y'}{x} - \left( \beta^2 + \frac{m^2 - y^2}{x^2} \right) y = 0. \quad (A.9) \]

This shows that \( y \) as given by Eq. (A.1) does indeed satisfy the required differential equation.

**A.2 FD Mesh Refinement Study**

For investigating the effect of the grid Fourier number \((Fo)\) on the accuracy of the numerical simulation, repeated code runs are performed with progressively larger number of through-thickness FD nodes. The setup described in EXP 2 of Chapter 3 is considered and the through-thickness temperature profiles obtained at locations 1, 2 and 3, at the instant the mould fills, are plotted in Figure A.1. The figure also contains the maximum grid Fourier number reached during the simulations. The observation that the different distributions compare very well leads to the inference that, at least for the present test case, the simulation accuracy is not significantly sensitive to the grid Fourier number.
A.3 Validation of the Simulation for a Non-planar Part

The accuracy of a non-isothermal filling simulation using the SUPG scheme is verified for a non-planar, hemispherical part with dimensions the same as those considered in Chapter 2, i.e. radius \( R = 0.1 \) m, part thickness \( h = 4.7 \) mm and fibre volume fraction \( V_f = 0.37 \), which is injected at a constant rate of \( Q = 6.2 \times 10^{-6} \) m\(^3\)/s through a 3 mm radius gate located at its apex. The mould walls are however considered to be preheated to 75\(^\circ\)C while the fluid is injected at 20\(^\circ\)C. The thermal properties of the materials are the same as those provided in Table 3.2.

While deriving the analytical solutions it is again assumed that the temperature within the mould eventually reaches a steady-state if the fluid is continuously injected post complete mould filling. This is indeed found to be the case while analysing the simulation results. Therefore, the energy equation is written in a normalized form in a spherical coordinate system as,

\[
\frac{\rho c_p Q}{2 \pi R^2 h k \sin \theta} \frac{\partial \theta}{\partial \theta} = \frac{\partial^2 T}{\partial \theta^2},
\]  

(A.10)

where \( \theta \) is the polar angle. Note that in Eq. (A.10) the in-plane diffusion is ignored for the sake of simplicity. Moreover, the normalization of the temperature is done as follows,
On applying the variable separation method the general solution for the dimensionless temperature is found to be,

\[ \hat{T} = \sum_{n=1}^{\infty} c_n e^{-\frac{2\pi^2 n^2 R^2 k \cos \theta}{\rho r c_p q h}} \sin \frac{n \pi z}{h}. \]  \hspace{1cm} (A.12)

Here \( c_n \) is evaluated from the Fourier expansion of the boundary condition at the injection gate, which gives,

\[ c_n = \frac{2(\cos n \pi - 1)}{n \pi} e^{-\frac{2\pi^2 n^2 R^2 k \cos \theta_{inj}}{\rho r c_p q h}}. \]  \hspace{1cm} (A.13)

The derived analytical solution is used to test the accuracy of the simulation at three points inside the mould; \( \theta = 15^\circ \) (location 1), \( 30^\circ \) (location 2) and \( 60^\circ \) (location 3). The results, as displayed in Figure A.2, show excellent agreement between the analytical solutions and the numerical predictions.

![Graphs showing comparison of analytical and numerical predictions](image-url)

Figure A.2: Comparison of analytical and numerical predictions for through-thickness temperature profiles at three reference points.