

Titre: Modeling of Transitional Flows on Roughened Surfaces for Icing Applications
Title:

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Author:

Date: 2022

Type: Mémoire ou thèse / Dissertation or Thesis

Référence: Blanchet, M. (2022). Modeling of Transitional Flows on Roughened Surfaces for Icing Applications [Mémoire de maîtrise, Polytechnique Montréal]. PolyPublie.
Citation: <https://publications.polymtl.ca/10714/>

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URL de PolyPublie: <https://publications.polymtl.ca/10714/>
PolyPublie URL:

Directeurs de recherche: Éric Laurendeau
Advisors:

Programme: Génie aérospatial
Program:

POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

Modeling of Transitional Flows on Roughened Surfaces for Icing Applications

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Département de génie mécanique

Mémoire présenté en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

Génie aérospatial

Décembre 2022

POLYTECHNIQUE MONTRÉAL

affiliée à l'Université de Montréal

Ce mémoire intitulé :

Modeling of Transitional Flows on Roughened Surfaces for Icing Applications

présenté par **Maxime BLANCHET**

en vue de l'obtention du diplôme de *Maîtrise ès sciences appliquées*

a été dûment accepté par le jury d'examen constitué de :

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DEDICATION

*To my friends and family,
who have always been there for me. . .*

*À mes amis et ma famille,
qui ont toujours été là pour moi. . .*

ACKNOWLEDGEMENTS

The research work described in this master thesis is part of a project funded by a Bombardier/NSERC Collaborative Research and Development (CRD) grant. This work is supported in part by NSERC, CRIAQ, and FRQNT. Calculations were performed on Compute Canada/Calcul Quebec clusters.

I would like to thank my supervisor, Prof. Éric Laurendeau, who guided me during this project, overcoming the difficulty due to the pandemic and remote work. He was able to supervise me brilliantly while giving free rein to my scientific mind and providing me with opportunities, such as an internship at TU Braunschweig and participation in a conference.

I am also grateful to the members of the Advanced Aerodynamics department at Bombardier implicated in the project, in particular Guy Fortin. The weekly meetings and exchanges we had while analyzing results were very helpful to guide my project and to improve my understanding of the icing phenomena as a whole.

Finally, I want to express my thanks to my lab partners at Polytechnique Montreal. A special thanks to Simon for his advice and support on icing and Frederic for his help with the transition model and his formative approach to improving my coding skills.

RÉSUMÉ

Le givrage est de la plus haute importance dans le domaine de l'aéronautique, d'une part puisqu'il demeure dans son ensemble assez incompris, et de l'autre puisqu'il existe des requis complexes de certification aéronautique liés au givrage des pièces composant les aéronefs. Suite à plusieurs accidents, ces normes requièrent maintenant de prédire les géométries de glaces qui peuvent s'amonceler sur des appareils soumis à des conditions de givrage critiques. Sous ces conditions, différents types de glace peuvent s'accumuler sur les surfaces de l'avion, comme du verglas ou des cristaux de glace qui, selon le cas, se traduisent par des géométries complexes qui affectent drastiquement les performances de vol. Pour modéliser et prédire ces formes de glace, des tests expérimentaux sont effectués, mais des outils et modèles numériques de plus en plus complexes sont aussi utilisés. Par contre, en se rapprochant de la température de fusion de l'eau, un film d'eau peut se créer et divers mécanismes liés au givrage entrent alors en jeu. Ces mécanismes plus complexes sont difficiles à modéliser et on remarque une perte de précision des outils prédictifs pour la glace de type verglas. Des modèles plus physiques doivent alors être ajoutés aux codes de givrage actuels afin d'améliorer les prédictions et de répondre aux plus récentes normes de certification.

L'objectif de ce projet de recherche est d'améliorer les prédictions des formes de glace de type verglas, apparaissant à plus hautes températures, sur des aéronefs soumis à diverses conditions de vol. Afin de répondre à cet objectif, une modélisation plus proche de la physique des phénomènes entourant le givrage a été ajoutée dans le logiciel maison CHAMPS, correspondant aux standards actuels des codes de givrage de seconde génération. Les formes de glace sont obtenues en employant en séquence divers modules: un module pour l'aérodynamique, un module pour l'accumulation de gouttelettes, un module pour les échanges thermodynamiques de surface et un module pour l'évolution de la structure de glace. L'aérodynamique est identifiée comme étant le module pouvant être amélioré et deux composantes principales ont été implémentées : la prédiction de la transition laminaire turbulente de la couche limite et la modélisation de la rugosité locale de glace. Ces deux phénomènes influent directement le transfert de chaleur convectif permettant le givrage. Les formes de glace obtenues sur des cas analysés dans le tunnel de recherche de givrage NASA Lewis ont été étudiées en considérant les modèles de façon conjointe. Le givrage étant un phénomène disparate et peu reproductible, certains ont examiné l'effet d'un modèle stochastique sur les formes de glace obtenues, en plus des modèles suggérés dans ce travail.

Premièrement, l'écoulement aérodynamique est simulé par un solveur des équations moyennées de Reynolds en volumes finis. Les modèles de turbulence utilisés par CHAMPS sont vérifiés et validés, car ils servent de base au développement des nouvelles méthodes précédemment énumérées. Des équations de transport supplémentaires, permettant de prédire la transition laminaire turbulente, sont ensuite ajoutées aux modèles de turbulence actuels. Cela permet d'obtenir une représentation plus physique de la couche limite à la paroi du profil. Cette dernière influence directement le transfert de chaleur convectif qui affecte le gel de la glace. Les équations de transition sont vérifiées en comparant à des valeurs du coefficient local de friction obtenues par tests de soufflerie sur des profils standards.

Deuxièmement, différents modèles de rugosité sont introduits i) pour représenter l'état de surface de la glace s'accumulant sur les géométries et ii) pour augmenter le transfert de chaleur convectif sur la surface initiale. Une rugosité uniforme basée sur la hauteur équivalente en grains de sable est d'abord proposée, correspondant à la méthode usuellement utilisée en recherche et en industrie. Elle est ensuite couplée aux équations de transition en employant une équation de transport de rugosité qui déplace le point de transition en amont de l'écoulement selon la hauteur de rugosité. Le transfert de chaleur associé à une hauteur de rugosité est vérifié en comparant à des résultats numériques de codes bien établis. L'effet des modèles sur les formes de glaces obtenues est étudié sur des cas expérimentaux. Les résultats montrent qu'une région de laminarité est parfois captée par les modèles, modifiant la forme de glace recueillie. Par contre, le fait d'imposer une valeur unique de rugosité pourrait déclencher la transition trop près du point de stagnation.

Troisièmement, des modèles permettant de déterminer localement l'amplitude de la rugosité de surface sur la géométrie de glace sont implémentés. Ces derniers sont étalonnés en recourant à des variables locales connues des différents modules du solveur, à partir de résultats expérimentaux de formes de glace et de rugosité. Les effets de ces modèles sur une série de cas de givrage bidimensionnels sont étudiés, de même que le couplage avec le modèle de transition récemment implémenté. L'utilisation de tels modèles permet d'ajuster la rugosité pour chaque couche de glace et de modifier le transfert de chaleur convectif, ce qui a pour effet de déplacer la position et l'orientation des cornes de glaces simulées. Les résultats montrent que la rugosité de surface calculée est faible dans la région du film d'eau, ce qui déclenche la transition laminaire turbulente plus loin du point de stagnation, donnant des géométries de glace davantage alignées avec l'expérimental par rapport aux modèles de rugosité globale.

Pour conclure, différents modèles ont été implémentés dans CHAMPS pour raffiner la prédiction de l'écoulement aérodynamique pour des cas de givrage, améliorant le calcul du transfert de chaleur et les simulations de formes de glace. Les effets des modèles de turbulence et de transition, ainsi que ceux des modèles de rugosité globale et locale sont observés sur les cas bi-dimensionnels provenant de résultats expérimentaux. De plus, ces extensions n'affectent pas la structure déjà établie des codes de givrage et permettent de modéliser plus en détail la physique du processus d'accrétion de glace. Les résultats suggèrent que plus de données soient prises en compte pour étalonner les modèles de rugosité locale. Par contre, ces modèles ont un potentiel pour ajuster la forme et l'orientation des cornes de glace simulées. Un modèle de densité locale et des effets stochastiques pourraient être ajoutés aux processus, afin de simuler les porosités et les plumes de glace par exemple.

ABSTRACT

Icing is of the utmost importance in the aeronautical field since it remains rather misunderstood and there are complex certification requirements related to the icing of aircraft components. Following several accidents, these standards now require the prediction of ice geometries that can accumulate on aircraft subjected to critical icing conditions. Under these conditions, different types of ice can agglomerate on the aircraft surfaces, such as ice crystals or glaze ice. Depending on the case, this can lead to complex geometries that drastically impact flight performance. To model and predict these ice forms, experimental tests are performed, but complex numerical tools and models are also used. On the other hand, when approaching the melting temperature of the water, a film can be created and various mechanisms related to icing come into play. These more complex mechanisms are difficult to model and a loss of accuracy of the predictive tools is noticed. More physical models must then be added to the current icing codes to improve the predictions and meet the latest certification standards.

The objective of this research project is to improve the prediction of glaze ice shapes, appearing at higher temperatures, on aircraft subjected to various flight conditions. To meet this objective, more physical modeling of the phenomena surrounding icing has been added to the in-house software CHAMPS, corresponding to the current standards of second-generation icing codes. The ice shapes are obtained by using various modules in sequence: a module for aerodynamics, a module for droplet accumulation, a module for surface thermodynamic exchanges and a module for ice structure evolution. Aerodynamics is identified as the module that can be improved and two main components have been implemented: the prediction of the laminar-turbulent boundary layer transition and the modeling of the local ice roughness. These two phenomena directly impact the convective heat transfer allowing icing. The ice shapes obtained on cases analyzed in the NASA Lewis Icing Research Tunnel have been studied by considering the coupled effect of the models. As icing is a chaotic and poorly reproducible phenomenon, some have examined the effect of a stochastic model on the resulting ice shapes, in addition to the models suggested in this work.

First, the aerodynamic flow is simulated by a finite volume Reynolds-averaged Navier–Stokes solver. The turbulence models used by CHAMPS are verified and validated, as they serve as a basis for the development of the new methods listed above. Additional transport equations to predict the turbulent laminar transition are then added to the current turbulence models. This allows the obtention of a more physical representation of the boundary layer at the wall

of the airfoil. This has a direct influence on the convective heat transfer that impacts the freezing of the ice. The transition equations are verified through comparisons with values of the local friction coefficient obtained by wind tunnel tests on standard wing shapes.

Secondly, different roughness models are introduced i) to represent the surface of the ice accumulating on the geometries and ii) to increase the convective heat transfer on the clean surface. A uniform roughness based on the equivalent sand grain height is first proposed, as it is usually used in research and industry. It is then coupled to the transition equations by a roughness transport equation that moves the transition point upstream according to the roughness height. The heat transfer associated with a roughness height is verified through comparison to well-established numerical code results. The impact of the models on the obtained ice shapes is studied with experimental cases. The results show that a region of laminarity can be captured by the models, modifying the ice shapes. On the other hand, imposing a unique roughness value could trigger the transition too close to the stagnation point.

Thirdly, models are implemented to determine locally the amplitude of the surface roughness on the ice geometry. These models are calibrated using experimental results of ice shapes and roughness, employing local variables computed by the different modules of the solver. The effects of these models on a series of two-dimensional icing cases are studied, as well as the coupling with the recently implemented transitional model. The use of such models allows for the adjustment of the roughness for each ice layer and for the heat transfer to be altered, thereby shifting the position and orientation of the simulated ice horns. The results show that the calculated roughness is low in the water film region, which triggers the turbulent laminar transition further away from the stagnation point, yielding ice geometries that are more aligned with the experimental compared to the global roughness models.

To conclude, different models have been implemented in CHAMPS to refine the prediction of the aerodynamic flow for icing cases, improving the heat transfer calculation and ice shape simulations. The impacts of turbulence and transitional models, as well as global and local roughness models, are studied with two-dimensional experimental results. Moreover, these extensions do not affect the already established structure of the icing codes and allow to model more physics in the ice accretion process. The results suggest that more data should be considered to calibrate the local roughness models. However, these models have the potential to adjust the shape and orientation of simulated ice horns. A local density model and stochastic effects could be added to the processes to simulate porosities and ice feathers for example.

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LIST OF SYMBOLS AND ACRONYMS

General symbols

ΔT_{0S}	Stagnation supercooling temperature	[K]
A_r	Roughness Amplification variable	[—]
c	Reference chord length	[m]
C_f	Local friction coefficient	[—]
c_p	Specific heat capacity at constant pressure	[J/(kgK)]
d	Wall distance	[m]
h_{ice}	Predicted ice height	[m]
k	Turbulent kinetic energy	[m/s ²]
k_c	Thermal conductivity	[W/(mK)]
k_s	Equivalent sand grain roughness	[m]
Ma	Mach number	[—]
$\vec{n}$	Grid unit normal	[—]
p	Pressure	[Pa]
Pr	Prandtl number	[—]
Pr_t	Turbulent Prandtl number	[—]
q	heat flux	[W/s ²]
$\dot{Q}$	Energy rate	[Pa]
Re	Reynolds number	[—]
$Re_{\theta t}$	Transition momentum thickness Reynolds number	[—]
Re_{ks}	Roughness Reynolds number	[—]
R_q	Root-mean-square of the roughness scale	[—]
$\tilde{Re}_{\theta t}$	Transported transition momentum thickness Reynolds number	[—]
s	Curvilinear distance from the leading edge	[m]
T	Temperature	[K]
Tu	Freestream turbulence intensity	[%]
t	Physical time	[s]
U	Velocity norm	[m/s]
u_i	Velocity component in i-direction	[m/s]
x	Normal distance to the leading edge	[m]
x_i	Cartesian coordinates in i-direction	[m]
y	Wall normal distance	[m]

Greek symbols

β	Collection efficiency of the droplets	$[-]$
γ	Heat capacity ratio of air or Intermittency	$[-]$
η	Freezing fraction	$[-]$
μ	Dynamic viscosity	$[kg/(ms)]$
ν	Kinematic viscosity	$[m^2/s]$
$\tilde{\nu}$	Spalart-Allmaras variable (mod. eddy viscosity)	$[m^2/s]$
ρ	Density	$[kg/m^3]$
τ	Shear stress	$[Pa]$
ω	Specific turbulence dissipation rate	$[1/s]$

Subscripts and Superscripts

∞	Freestream property
0	Initial/Clean value
+	Non-dimensionalised in inner region
<i>conv</i>	Convective
<i>ice</i>	Ice property
<i>l</i>	Laminar value
<i>rec</i>	Recovery value
<i>ref</i>	Reference value
<i>t</i>	Turbulent value
<i>tot</i>	Total value
<i>wall</i>	Wall value

Acronyms

AIAA	American Institute of Aeronautics and Astronautics	
AoA	Angle of Attack	
CHAMPS	Chapel Multi-Physics Software	
CFD	Computational Fluid Dynamics	
D	Dimension	
FAA	Federal Aviation Administration	
HTC	Heat Transfer Coefficient	
IPW1	First AIAA Ice Prediction Workshop	
IRT	Icing Research Tunnel	
LRC	Langley Research Center	
LTPT	Low Turbulence Pressure Tunnel	
LWC	Liquid Water Content	$[g/m^3]$

MVD	Median Volume Diameter	[<i>m</i>]
NASA	National Aeronautics and Space Administration	
NS	Navier-Stokes	
PDE	Partial Differential Equation	
RANS	Reynolds-Averaged Navier-Stokes	
SA	Spalart-Allmaras	
SST	Shear Stress Transport	
SLD	Supercooled Large Droplets	

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CHAPTER 1 INTRODUCTION

This chapter defines the context, the certification requirements and the numerical state-of-the-art of ice accretion predictions which lead to the problem statement of the present work. The importance of the heat transfer assessment for numerical simulations is emphasized and, based on these observations, the thesis objectives and outline are established.

1.1 Context

Contamination of aircraft surfaces (i.e ice, bugs) must be taken into consideration during the aircraft design cycle. Indeed, certification requirements quantify specific aircraft characteristics toward the possible loss of lift, increase in drag or change in the pitching moment. Factors can lead to the contamination of an aircraft's skin, the primary source being ice accretion. As an airplane flies into clouds, water droplets below $0^{\circ}C$ can impinge on the surfaces, exchanging heat with the surface and the environment and transforming into ice [7]. It reshapes the surfaces of the plane and impacts its aerodynamic properties as it reduces its maximum lift and increases its drag [8]. This can lead to a rapid decline of the altitude that can endanger passengers, as shown by an accident that occurred in December 1997 with Air Canada Flight 646 from Toronto to Fredericton. In difficult weather, the wing had accumulated ice, reducing its performance, and, in combination with other factors, resulted in the accident [9].

1.2 Certification requirements

Aeronautical certification organizations, such as the Federal Aviation Administration (FAA), the Canadian Aviation Regulations (CAR), or the European Aviation Safety Agency (EASA) established requirements for airplanes operating in a flight envelope containing icing conditions. For example, FAA Part 25 [10] requires that by the mean of analysis and/or tests, an applicant must show that an airplane can function safely in the flying envelope by showing supporting data that critical lifting surfaces and accessories such as the cooling intakes, the antennas, the propellers, the windshield, etc, will stay free of ice and/or that the airplane can still fly in these iced conditions.

To specify the engineering requirements for atmospheric icing, Appendix C and O of FAA Part 25 state two envelopes to assess the maximum/critical conditions that can be encountered. These envelopes define the Liquid Water Content (LWC), the water droplet size and the air

temperature. Currently, icing wind tunnel experiments are being carried out to anticipate the form of ice generated under Appendix C and O conditions. In these facilities, engine air intakes, wing components, rotors and propellers are put under icing conditions. These tests are very long and costly. Flight tests are also used, equally long and costly with the added risk of the loss of the aircraft and its crew. This explains why numerical simulations are more and more used as complementary analysis and design tools [11].

1.3 Numerical modeling of ice accretion

To certify an airplane, one way to obtain the necessary data to assess the aircraft performance under Appendix C and O conditions is to predict numerically the ice accretion in these conditions at normal operating speeds of an aircraft. The worst ice shape degrading the aircraft performance is obtained and the effects on the aerodynamic properties are investigated. The goal is to demonstrate that a minimum level of maneuverability and performance of the aircraft will be attained. To obtain a specific ice shape (i.e. accretion) different numerical modules need to be used. These modules must allow computing the flow trajectory around an airplane, the droplet path to see which are impacting the aircraft surface and the shape of the cumulated frozen droplets. The final ice shape is then physically produced and tested in tunnels to assess the impact on the performance of the aircraft. The numerical simulation of the region where ice accretes also helps to determine the position of the ice protection captors and anti-icing systems.

The aerodynamic part is easily computed with conventional numerical fluid dynamics tools. The droplet part is more complex, as the impingement rate of the droplets on the surface must be taken into account. The thermodynamic part is even more burdensome, as different types of ice can accumulate on the aerodynamic surfaces, depending on the heat transfer between the surface and the environment. This thermodynamic balance is then used to obtain the geometry. More details are given in Chapter 2. Many uncertainties remain, as the final ice shape relies on a multitude of parameters, most of them being defined by Federal Airworthiness Regulations (FAR) Appendix C and O, but others coming from the numerical models.

1.4 Problem statement

Supercooled water droplets accumulating on aerodynamic surfaces can be of several types. The first type is ice generated under rime icing conditions. Under this type of icing condition, the most frequent type of ice is streamwise ice where all of the impinging water droplets

freeze upon impact with the geometry, creating an agglomeration [12]. Another category for unswept wings is roughness ice. With this type of ice, a smooth and thin layer of rime ice assembles on the leading edge of the geometry and narrow spikes of ice, called feathers, arise past the ice layer region, modifying the local surface roughness [12]. Rime cases are predicted with low uncertainties since no matter the local value of the heat transfer, all the water freezes. However, under glaze icing conditions, only a fraction of the impinging water droplets freezes upon the impact depending on the local heat transfer, which is the main component affecting the energy balance at the surface. The rest of the water, unfrozen, travels downstream and may freeze during its runoff. As shown in Figure 1.1, a glaze ice geometry is more complex, since the water film freezes during its runback, creating horns of ice. It significantly affects the aerodynamic performance of an aircraft by increasing the pressure drag behind these ice formations. The second type of glaze ice for unswept wings is the spanwise ridge ice. This type of ice arises when the leading edge is protected and the water cannot freeze. The film flows up and freezes, creating ridges in unprotected zones [12]. A mixed combination of rime and glaze ice can also appear. Thus, for numerical predictions of ice shapes, an accurate value of the heat transfer must be used at the wall to correctly predict the film region and the final ice shape on an aircraft surface.

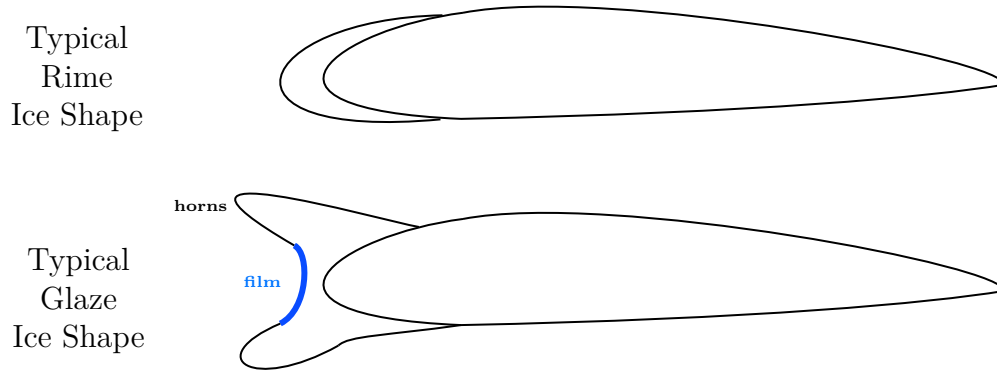


Figure 1.1 Typical rime ice shape and glaze ice shape on a schematized airfoil

An empirical prediction of the heat transfer was used in the first-generation aero-icing software, which employed panel methods, boundary-layer codes and Lagrangian droplet modules. The second-generation aero-icing software, which employ Reynolds-averaged Navier–Stokes (RANS) equations, now compute directly the heat transfer at the wall using a numerical solution of the flow field. Yet, these models are still in development and might use objectional approximations while computing the convective heat transfer. For example, it is known that the flow regime impacts the value of the local convective heat transfer. Formulations for the

convective heat transfer exist for laminar and turbulent flow, and some might use an empirical relation to predict the flow transition. However, few researchers used transitional RANS models to compute the transition location and improve the accuracy of the heat transfer as well as the computed shear stress.

Moreover, while it is commonly assumed that a numerical roughness must be imposed on a lifting surface to account for the initial phase of ice accretion that consists of rough ice, the majority of the second-generation icing codes use a global value for the roughness, considering a uniform and homogeneous distribution. This increases globally the heat transfer at the wall. However, recent experimental results concerning ice shapes have shown that the roughness greatly changes along an iced lifting surface, where the value is low in the film region and higher in the rivulets/beads region. The modelization of the local surface roughness is important since even if most of the ice features are captured through the mesh, the microscopic properties of the ice surface are not taken into account. This has an impact on the flow and this is why several local roughness models exist to predict the value along a certain geometry depending on the icing conditions, although these models contain their share of uncertainties. Some are based on ice accretion physics but are not robust enough, while others have been calibrated using flow variables but only with a limited number of cases.

1.4.1 Heat transfer assessment

For the prediction of ice accretion, an important aspect to take into account is the convective heat transfer between the surfaces prone to ice accretion and the surrounding air. In the industry, many use integral boundary layer equations to calculate the heat transfer coefficient. This computed heat transfer coefficient depends on multiple factors such as the temperature of the surface, the temperature of the fluid near the surface, the roughness of the surface, etc [13]. Even if a heat transfer coefficient can be computed on the surface, there is a lack of procedures for the validation of the codes. Different databases have been created in 2D, with diverse icing conditions to provide a pool of comparison data in different icing regimes (cold rime, rime-to-glaze transition regime, and warm glaze ice). For hot cases, the heat transfer can affect drastically the final ice shape, since it regulates whether or not the water film freezes at a specific location on the ice shape surface. In 3D, ice-shape data have been extracted for icing cases. However, since the capabilities of the software are not yet sufficient in 2D, attempts to simulate the 3D ice shapes form a relatively recent research topic as exemplified by the 2019-2024 ICE GENESIS international projects [14] that examine 3D modeling.

1.5 Research objectives

This research project aims to improve the accuracy of the software-predicted ice shapes, focusing on heat transfer modeling for realistically ice-roughened surfaces. The specific objectives are:

1. Investigate the impact of several turbulence/transitional models on the icing workflow;
2. Develop a new model that takes into account the simultaneous effects of the flow transition and the wall roughness to evaluate the flow field;
3. Investigate the impact of the newly created model on the prediction of ice shapes.

While a vast majority of current icing simulations use a turbulence model, few have studied the effect of the choice of the model on the predicted ice shapes. At the moment, new RANS models are being created, but the best practices still suggest using the same previous turbulence models. The first objective will permit the determination of the best practices for the selection of the turbulence model during an icing simulation. The second objective will allow the integration of the microscopic roughness effects of the ice in the simulations, coupled with a model that can capture the flow transition to fully capture the effect of the newly modeled roughness. Finally, the third objective will make it possible to determine if the newly implemented models improve the ice shapes prediction in comparison with standard results from the literature.

1.6 Thesis outline

Chapter 2 introduces the literature review relevant to the turbulence modeling, the icing simulations and the consideration of the surface roughness related to heat transfer. Then, Chapter 3 presents the implementation, verification and validation of the turbulence and transitional models in the icing software CHAMPS. The models and results on conventional airfoil cases are presented to assess CHAMPS accuracy. Results are also displayed on different grid sizes to show the grid convergence of the discretized models. Chapter 4 describes diverse roughness models that can be paired with these turbulence and transitional models. The effect of a global roughness on the transition location is also shown in Chapter 4, as well as rime and glaze ice cases. Chapter 5 analyzes different local roughness models and their impacts on the ice shapes. Results and effects on ice shapes are discussed. Finally, Chapter 6 provides an overview of the research project and exposes the current difficulty encountered. Propositions of further developments for aero-icing software are also discussed.

CHAPTER 2 LITERATURE REVIEW

This chapter presents the review of the icing workflow for first and second-generation icing software and their respective assumptions. The solvers' fundamental equations are defined and the modeling challenges of the turbulence, the heat transfer and the different types of ice roughness are described. Diverse methods are available to introduce the roughness in icing codes, such as a global uniform roughness model or a local roughness model. Regarding these topics, conclusions of the First American Institute of Aeronautics and Astronautics (AIAA) Ice Prediction Workshop are brought out.

2.1 Icing workflow

Different approaches exist to model the ice accretion on aerodynamic surfaces in icing conditions. Still today, two-dimensional capabilities are the norm for icing software, since several problems still appear in three-dimensional simulations, specifically for re-meshing. While some distinctions appear between icing codes, they globally all use the same steps within a quasi-steady approach. Some popular icing codes of the first generation and their properties are presented in Table 2.1.

Table 2.1 General properties of the first-generation aero-icing software [1]

Code	Developer	Flow Solution	Droplet Trajectory Tracking	Thermodynamic Model	Heat Transfer	Multi Step	Roughness Correlation	Droplet Distribution	3D Possible
ONERA-2000 code	ONERA	Potential Equation	Lagrangian	Messinger	Correlation	YES	YES	?	NO
Multi-Ice	CIRA	Panel Method	Lagrangian	Messinger	?	YES	?	Possible	NO
HELICE	CIRA	Multiple Interface	Lagrangian	Messinger	Integral Method	NO	?	Possible	YES
TRAJICE2	DERA	Panel Method	Lagrangian	Modified Messinger	Correlation Integral Method	YES	YES	NO	NO
CANICE	Polytechnique Montréal	Panel Method	Lagrangian	Modified Messinger	Integral Method	YES	?	?	NO
LEWICE 2.0	NASA Glenn Research Center	Panel Method	Lagrangian	Modified Messinger	Integral Method	YES	YES	Possible	NO

Other codes of the second generation include LEWICE 3.0 [15] developed by NASA, ONICE 2D/3D [16] and IGLOO 2D [17] developed by ONERA and FENSAP-ICE developed by Numerical Technologies International [18]. In Montreal, NSCODE-ICE [19] from Polytechnique Montreal, CANICE_BA [20] from Bombardier and CHAMPS [4], a new aero-icing software at Polytechnique Montreal, are used. The ice accretion simulations typically consist of six typical stages [21]:

1. Generation of a mesh to be used by the different modules;
2. Determination of the aerodynamics associated with the geometry (flow module);
3. Computation of the distribution of the supercooled water droplets impinging on the geometry (droplet module);
4. Evaluation of the freezing rate and the freezing fraction of the impinged water droplets on the body (thermodynamic air-water-surface module);
5. (Optional) Re-meshing of the interface with the new ice shape and the field for a multilayer purpose;
6. Assessment of the final ice shape accumulated on the body (geometric module).

Each software uses these steps to compute the ice shape accumulating in specific conditions. The codes differ by how each module works and computes the solution. Specific details linked to each module will be presented in the following sections, considering them uncoupled. Other approaches also exist where the modules are fully coupled [22, 23] or where stochastic approaches [24, 25] are used. These approaches consist of a Lagrangian method for the droplets and accumulating the ice discretely on a cartesian lattice to generate stochastically complex glazed ice shapes, such as feathers. Figure 2.1 schematizes how the modules are linked when they are uncoupled. When computing the flow field around a body, several approaches are available. One can employ the panel method, giving a potential flow solution, or methods using a spatial grid around the geometry (full potential or Euler/RANS methods) [26]. The flow solution is used to determine the droplet trajectories by an Eulerian or Lagrangian approach, the RANS equations give a proper resolution of the boundary layer and also provide the convective heat transfer at the surface for the freezing mechanism. While the panel method approach has the advantage of being computationally cheaper and of simplifying the re-meshing, it has issues when the geometry is complex (like multi-element airfoils) or when the flow is separating. Moreover, the convective heat transfer cannot be extracted from panel method codes. For RANS codes, the computation is more expensive but allows for more complex geometries and flow conditions.

Several hypotheses are made in the droplet solver. The droplets are assumed small enough to not disturb the flow. It is considered that gravity and drag are the only forces affecting the droplets. Methods exist for larger droplets, but they are not treated in this work. Two methods are applicable when evaluating the droplet trajectories with the flow solver. A Lagrangian particle tracking method integrates the trajectories of each droplet separately from its seeding point to its impingement on the geometry. A process or the user determines

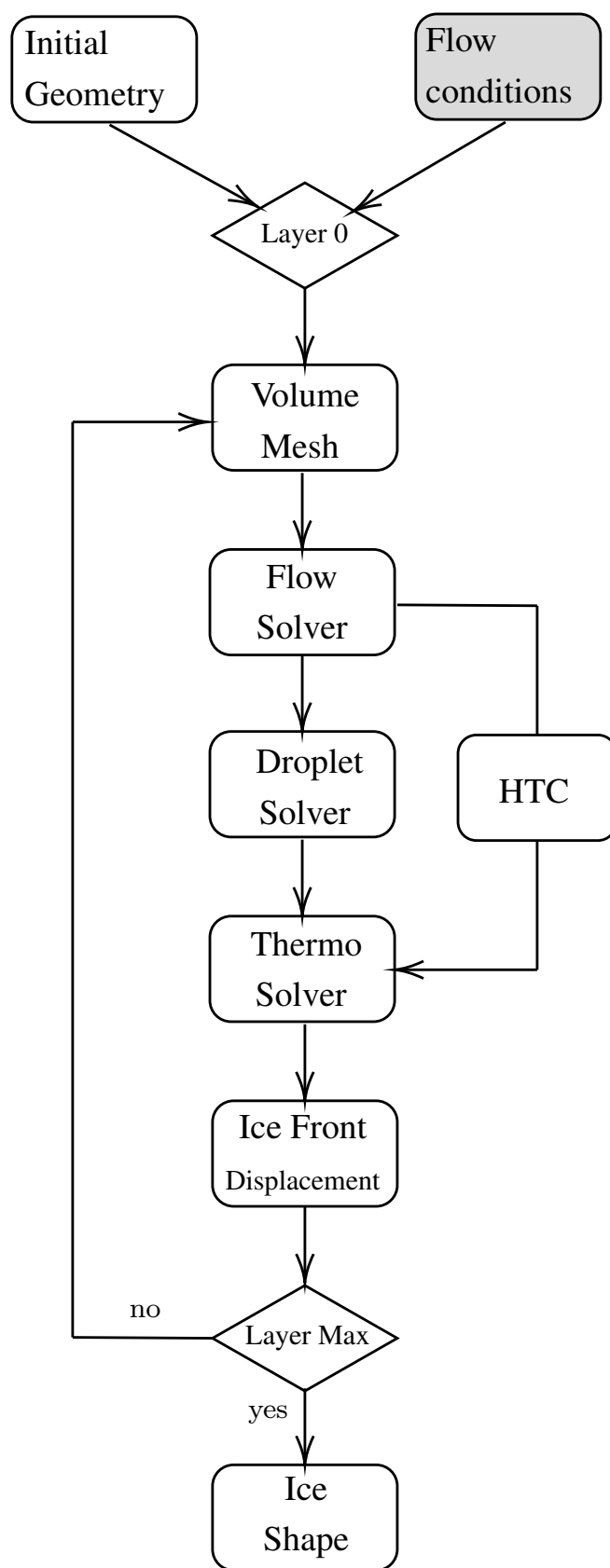


Figure 2.1 CHAMPS icing workflow

the range of the seeding points needed to obtain the impingement limits on the geometry [27]. This technique was employed in the first-generation icing codes. With an Eulerian approach, the droplet properties (density or mass fraction, and velocities) are solved in each cell of the grid utilized for the RANS solver with the same numerical techniques. Since the solution is known in the field, the impingement limits do not need to be computed. This process has been used by several icing software like FENSAP-ICE [18]. Many size distributions can be handled for the water droplets and the impingement on the geometry is obtained with a weighted sum.

To compute the shape of the frozen water on the geometry surface, the fraction of the water that freezes on the surface as well as the water runback need to be assessed. To do so, a thermodynamic solver is employed. The Messinger model analyzes the heat and mass balance at every cell on the surface to compute the ice growth. The surface mesh is generally used, where a control volume is defined [19]. For each cell, the evaluated fluxes consist in:

- The convective heat transfer (from the flow solver);
- The evaporation/sublimation;
- The heating of the impacting water;
- The cooling or heating of the running water from a neighboring surface;
- The cooling of ice;
- The latent heat of the freezing water.

Different thermodynamic models are available to compute the ice geometry. In NSCODE-ICE, four different models have been implemented: Messinger, iterative Messinger, extended Messinger by Myers [28] and shallow water icing models. Each of these algebraic and Partial Differential Equations (PDE) models has its strengths and weaknesses, as examined by Lavoie *et al.* [29].

The ice growth computed by the thermodynamic module is then used to compute the ice shape forming on the geometry, adopting different node displacement techniques. The surface mesh nodes are translated, in the direction of the cell normal, by the local ice thickness [30]. Unfortunately, mass conservation is not guaranteed with this technique when the geometry presents a succession of concave and convex features. This can also lead to a foldback of the geometry which prevents any further re-meshing. In these cases, limiters can be applied to limit the marching step of the geometry growth. Other techniques would be the use of

the Level-set method or a PDE formulation, which protects the simulation from a geometry foldback [31], or a hyperbolic mesh generation algorithm [32].

As the ice accretion mechanism is assumed to be a quasi-steady phenomenon, each module previously mentioned is executed in a steady state. However, the modified geometry has an impact on the flow field, which influences the droplet streamlines and thus the final ice shape accumulating on the body. The geometry evolution is affected by the icing time and might be generated in steps to improve the simulation accuracy. After an icing layer calculation, the surface mesh of the airfoil is deformed, then the volume grid is re-meshed. The multilayer process allows a gradual inclusion of the effect of the geometry on the other modules while conserving a steady state for each module computation. However, the multilayer procedure requires additional computations and introduces several risks, such as generating an invalid geometry with foldback or obtaining non-converging flow simulations.

2.1.1 Icing hypothesis

In view of the preceding information, the work will use standard hypotheses to facilitate the computation:

- The icing process is a quasi-steady phenomenon;
- The water droplets do not affect the airflow;
- The breakup, coalescence and collision of the water particles are negligible.

The first hypothesis means that each module is solved in a steady state, except for the geometry deformation. This is due to the fact that the flow physics time scale and the icing time scale are very different. Employing an unsteady approach would be time-consuming and the multilayer process is preferred to take into account the time-dependent nature of ice accretion. For the second hypothesis, since the mass loading of the droplets in the air is low, their effect on the flow is negligible and therefore, the flow equations do not need to be modified. For the third hypothesis, the droplets are considered sparse enough to neglect their interactions [33]. Splashing could be considered but this functionality is not yet available in CHAMPS.

2.2 RANS equations

The behavior of the flow and the heat transfer is governed by the RANS equations. This set of partial differential equations is based on the Navier-Stokes equations defined as, neglecting

the gravity terms [34]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0 \quad (2.1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (2.2)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_j} (\rho E u_j) = -\frac{\partial (p u_j)}{\partial x_j} + \frac{\partial (u_i \tau_{ij})}{\partial x_j} + \frac{\partial}{\partial x_j} \left(k_c \frac{\partial T}{\partial x_j} \right) \quad (2.3)$$

where the terms u_k are the velocities in the direction x_k for the spatial direction $k = 1, 2, 3$ in three dimensions. These equations are obtained from the conservation of mass, momentum and energy. The problem is that their analytical solutions only exist for specific and simple laminar canonical cases. For typical problems observed in industries, where the Reynolds number is high (of the order of a million) and the studied geometry is complex, they cannot be obtained. Therefore, numerical computations of these equations are necessary to assess turbulent flows which are composed of eddies of different time and length scales. Industries are using RANS formulations for icing applications, as more detailed models such as Large-Eddy Simulations (LES) or Direct Numerical Simulations (DNS) are too costly.

The RANS equations account for the turbulence in the Navier-Stokes equations by adding non-linear terms in the momentum equations to represent the momentum transferred by the eddies. These additional terms create a gap between the number of equations and the number of unknowns. This gap is called the closure problem. Additional assumptions need to be taken to pass through the nonlinearity of the Navier-Stokes equations in order to compute the solution [35]. One way is to use the Boussinesq Eddy-Viscosity assumption which is based on the premise that the convective transport of the turbulent momentum is similar to the molecular momentum transport. Creating the same effect as the molecular transport of momentum, it generates turbulent shear stress. The Reynolds stress tensor is therefore written in terms of the local mean strain rate of the flow and a turbulent viscosity, μ_t , now needs to be modeled as the only unknown:

$$\tau_{ij} + \frac{2}{3} \rho k \delta_{ij} = 2\mu_t \left(\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \quad (2.4)$$

It serves as a base for many of the RANS models that have been developed through the years. Near the wall, the normal gradients of the velocity are important. Assuming a zero-pressure gradient and y being normal to the wall, the shear stress at the wall is given by:

$$\tau_{wall} = (\mu + \mu_t) \frac{\partial u}{\partial y} \Big|_{y=0} \quad (2.5)$$

and the friction velocity is given by:

$$u_\tau = \sqrt{\frac{\tau_{wall}}{\rho_{wall}}} \quad (2.6)$$

Non-dimensional variables will be used for the next developments. They are defined by:

$$u^+ = \frac{u}{u_\tau}, \quad y^+ = \frac{yu_\tau}{\nu}, \quad \nu_t^+ = \frac{\nu_t}{\nu}$$

Eq. (2.6) can be written in terms of these non-dimensional variables:

$$(1 + \nu_t^+) \frac{du^+}{dy^+} = 1 \quad (2.7)$$

The inner region of the boundary layer can be decomposed into three subregions:

1. The viscous sublayer ($y^+ < 5$): The viscosity effects prevail, while the turbulence effects are low;
2. The buffet layer ($5 < y^+ < 30$): Viscosity effects and turbulence effects are present;
3. The logarithmic layer ($y^+ \geq 30$): The turbulence effects prevail;

The velocity profile given for these regions follows a semi-log plot as schematized in Figure 2.2. When roughness is applied, it adds viscous shear stress and Nikuradse [36] has shown that it leads to the translation of the logarithmic region of the profile by $-\Delta u^+$. Turbulence models try to replicate this shift.

2.2.1 Discretization and turbulence modeling

Several methods are currently being used by researchers and industries to take into account turbulent phenomena in external and internal flow solvers. In CHAMPS and other solvers, the aerodynamic flow field is solved with a finite volume unstructured RANS solver. The turbulence can be modeled with the Spalart-Allmaras (SA) one-equation model [37] or the SST k - ω two-equation model, and its variations [38]. Laminar-turbulent transition can be modeled with the transitional γ - $\tilde{Re}_{\theta t}$ equations model [39,40] coupled with either the Spalart-Allmaras model or the multiple variations of the k - ω model.

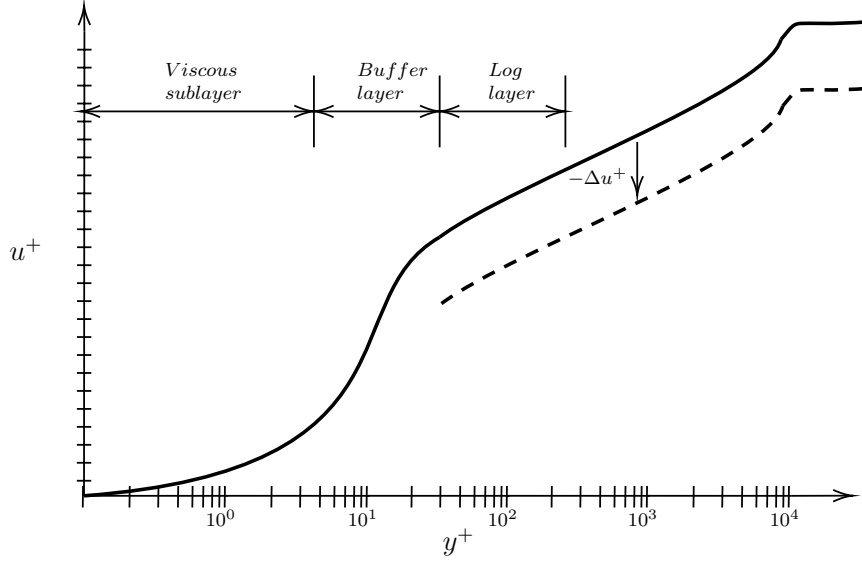


Figure 2.2 Velocity profile of the turbulent boundary layer with translation due to roughness

2.3 Heat transfer coefficient computation

The convective exchange at the wall is of great importance in icing because it is the most decisive energetic loss or gain term in the energy balance used to compute the ice shape. It is also the most difficult to obtain correctly. To evaluate the convective heat flux, it is necessary to determine the Heat Transfer Coefficient (HTC) and the recovery temperature. Several methods are available for the computation of the HTC. The icing software needs to be tuned to obtain the right value for this coefficient. Potential and inviscid flow models cannot be used to predict the HTC since no viscous effects are considered. Thus, the value must be parameterized based on the boundary layer characteristics [33]. This is called the Integral Boundary Layer (IBL) method [41,42] and different correlations can be employed in laminar and turbulent regions.

For RANS or boundary layer codes, when the skin friction is available, the convective heat transfer comes from the aerodynamic flow field and it is possible to avoid the integration process. The Reynolds analogy is used to retrieve the heat transfer coefficient from the skin friction coefficient enhanced by the surface roughness. The increase of the heat transfer is obtained by an increase in the wall turbulent shear stress with a correlation proposed by Kays and Crawford [43]. The goal here is to have a heat transfer that raises when the surface roughness increases. However, the value is strongly dependent on the choice of the turbulent model and the mesh near the wall defining the resolution of the temperature gradients. Different boundary conditions can be handled at the wall, passing from an adiabatic wall

condition to an isothermal wall condition, so the wall heat flux can be evaluated using the temperature gradient at the wall. Here, the different transitional models can be manipulated to predict either laminar or turbulent heat transfer. The convective heat transfer provided by Computational Fluid Dynamics (CFD) software for turbulent dry air is then converted to a heat transfer coefficient by dividing it by the difference between the airfoil temperature and the flow temperature [30].

To obtain the HTC, a first method employs Newton’s law of cooling with the difference between the imposed isothermal wall temperature, which is chosen by the coder or the user, and the farfield temperature. A second method is to use two flow solutions to improve the accuracy of the prediction of the heat transfer coefficient. Since the heat transfer coefficient depends weakly on the initial surface temperature distribution along the airfoil, it is evaluated with two arbitrary wall temperatures. The combination of the two wall temperature distributions leads to the final value of the heat transfer coefficient. This, however, adds a computational cost. A variant of this second method was proposed by ONERA [44]. It employs the recovery temperature instead of the isothermal wall temperature in the heat transfer coefficient computation. This accounts for compressibility effects, viscous dissipation as well as pressure gradient effects. The recovery temperature is unknown, so two solutions still need to be computed with two different wall temperatures. However, to reduce the computational costs, the recovery temperature can also be obtained from a theoretical relation [45].

2.4 Ice roughness qualification

Since the turbulent heat transfer computation for RANS codes is strongly based on the shear stress computed at the geometry surface, a roughness input must be imposed to increase the heat transfer and to physically represent the effect of the geometry. Roughness can appear in different forms on aerodynamic surfaces. It can be due to the surface finish or contaminant, the geometry of the initial body and particularly for this work: ice. The roughness caused by the ice accretion is dependent on the type of ice forming on the aerodynamic surface. Several types of ice can be present during the ice accretion process depending on the icing conditions as discussed in Section 1.3. The first type is rime ice, where the convective heat transfer is sufficient to freeze all the impinging droplets arriving on the surface. A second type is glaze ice, where the local heat transfer is insufficient to freeze all the incoming droplets, generating in some areas an unfrozen water film that runs back from the stagnation point and freezes in a horn shape. Beads and rivulets growing or being torn can be present on the surface [46]. Thus, depending on the freezing process, the roughness on the surface changes, where its height is minimal for the film and increases in the beads/rivulets regions [46].

The problem when assessing the roughness of the ice is that the convective heat transfer influences the freezing water behavior on the aerodynamic surface, as well as the size and positions of the freezing horns. This redefines the roughness computed. For this reason, a method to get out of this loop must be developed.

2.4.1 Global uniform roughness

While a few experimental data are available for the surface roughness on ice-accreted airfoils, most only use a global entry to impose a roughness on an aerodynamic surface. However, this unique value does not capture the true nature of the ice-shape roughness, which is not homogeneous. While deriving the logarithmic law, it is assumed that the flow closest to the wall is determined by viscosity. This is true only for hydrodynamically smooth surfaces, for which the average height of the surface roughness elements is less than the thickness of the viscous sub-layer. For a hydrodynamically rough surface, on the other hand, the rough elements are taller than the viscous sub-layer, leading to a wake formation behind each. It results in an increase in the shear stress at the wall. A roughness correction needs to be applied, depending on the roughness height at the wall, which shifts the velocity profile as observed in Figure 2.2. A rough surface may have a structured or random pattern and is composed of multiple length scales. Typically, RANS codes take into account an equivalent sand grain roughness, as proposed by Nikuradse [36] who studied the impact of a uniform-size sand grain roughness diameter on pipe flow. While there is still a challenge to transform usual surface roughness to an equivalent sand grain roughness, a majority of rough-wall measurements have been reported with this scale parameter and most of the roughness extensions for RANS models use it as an input [47].

Normally, the user gives his approximation of the roughness height. For a non-experimented user, this can lead to miscalculations in the final ice-shape geometry. This is why various methods have been developed to give an approximation of the global roughness to use. Shin *et al.* [48] suggest an empirical relation as a function of temperature, airspeed, LWC, Median Volume Diameter (MVD) and chord length. Han and Palacios [49] also have their formulation for the equivalent sand grain roughness based on the accumulation parameter (dimensionless ice accretion rate) and the freezing fraction at the stagnation point. Those correlations are obtained by using test databases and are not physics based. Because of the lack of experimental knowledge, ONERA uses a uniform roughness of 0.1 percent of the chord [50]. LEWICE 3.2 [42] uses a roughness formulation based on the freezing fraction at the stagnation point and is scaled using the leading edge diameter. Fortin *et al.* [51] proposed a correlation based on the supercooling temperature. The problem with these correlations is that they

all offer a different global roughness value for a specific test case. This is because they are based on different parameters and databases for their elaboration. Another problem is that a global value for the roughness might not hold for 3D cases. LEWICE 1.0 [52] employs an analytical relation established on the surface tension, the water viscosity, the water density, the surface shear stress and the wetted fraction of the surface. The computed roughness can also be multiplied by a factor to compare results with experimental data to account for higher turbulence levels in tunnels [52].

2.4.2 Local roughness

Recently, more and more local roughness models are being used. Fortin *et al.* [51] proposed a model based on the physics of the problem. It computes a film wave height, as well as beads and rivulets roughnesses based on the equilibrium of the forces at the surface. The prediction of this model is close to the experimental results. FENSAP-ICE [53] employs a roughness model based on rivulets properties, assuming a cylindrical shape for the elements and calculating the balance of the forces based on the analysis of the coalescence and dynamic equilibrium of supercooled water droplets. McClain *et al.* [6] proposed an empirical roughness model based on local surface parameters such as the freezing fraction, the local pressure coefficient, the local total temperature, the cloud properties and the cloud exposure time. These local variables are accessible from the flow, droplet and thermodynamic solvers. The height of the roughness enhances locally the convective heat transfer.

2.5 First AIAA Ice Prediction Workshop

Tremendous developments in the icing workflows and new acquisition techniques of experimental results led to the holding of the First AIAA Ice Prediction Workshop (IPW1) in July 2021. The goal of the workshop was to establish the current limits of 2D and 3D simulation capabilities in the ice accretion field by gathering different members of the community such as code developers and experimentalists. Rime and glaze ice conditions were defined on 2D and 3D, swept and non-swept, and single and multi-element geometries, based on available experimental data. Droplet distributions were also employed. Numerical results were compared to experimental data by analyzing the pressure coefficient, the droplet impingement on the surface, the convective heat transfer and the final ice shape. In order to assess the best practices and the state-of-the-art of the current icing simulation capabilities, the participants provided numerical data using different types of flow, droplet and thermodynamic solvers. Several observations were made a posteriori of the workshop, resumed below [3]:

1. Most of the participants used RANS models, such as the Spalart-Allmaras or the Menter $k-\omega$ SST turbulence models;
2. Several workflows adopted a global roughness model to enhance the convective heat transfer;
3. A very small proportion of the members employed laminar-turbulent models.
4. The droplet solvers used were a mix of Eulerian and Lagrangian approaches.
5. Out of 24 participants, only two utilized a local roughness formulation.

Results obtained from the workshop participants on different cases showed that no consensus has been reached for the best practices/modules to use. A lot of disparities are present between the participants when the final ice shapes are compared. Figure 2.3 displays the dissimilarities between the results of the workshop participants for case 242.

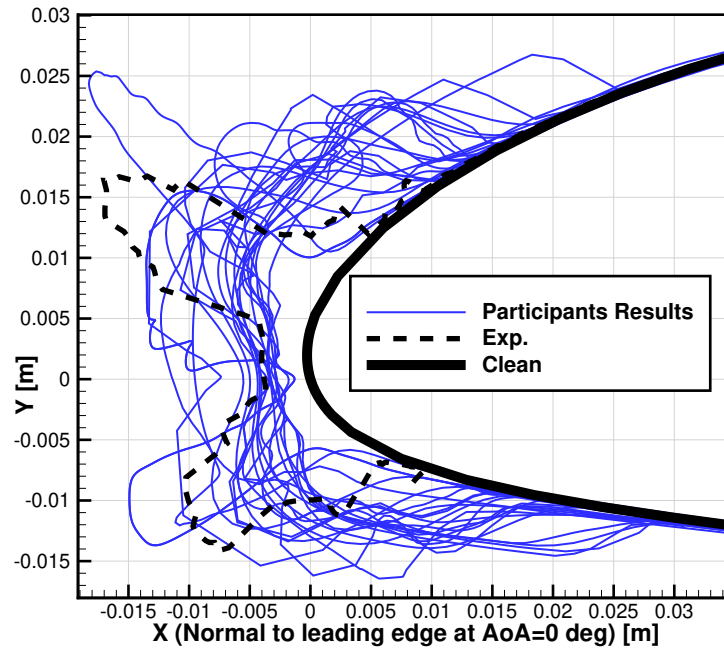


Figure 2.3 IPW1 participants ice shapes comparison for Case 242 [3]

From these observations, it is inferred that improvements still need to be made in icing software. Also, it is concluded that the icing workflow in CHAMPS is within the norms/best practices of the icing community [4]. While some attendees used transitional models instead of fully turbulent models and some employed a local roughness formulation instead of a global roughness formulation, no one has used them in an interrelated way.

CHAPTER 3 TURBULENCE COMPUTATION FOR HEAT TRANSFER

This chapter focuses on the implementation and the verification of the Spalart-Allmaras and k - ω SST turbulence models in CHAMPS. The evaluation of the HTC and the way it is affected by the turbulence models are discussed. To improve the heat transfer computation accuracy, a transition extension for these turbulence models is implemented and validated. However, limitations, assessed in Chapter 4, are still present for their use in the HTC computation.

3.1 Turbulence models

As shown in 2.2.1, the friction coefficient needs to be computed locally in the RANS code to avoid an integration process along the boundary layer. Since most of the flows present in icing conditions are under turbulent regimes, turbulence models need to be added to the flow module to compute the friction coefficient. These models increase the friction coefficient to a physically adequate value for turbulent flows. The Boussinesq assumption assumes a linear relationship between the Reynolds stress tensor and the turbulent eddy viscosity, which needs to be calculated from a turbulence model. These models are known as linear eddy viscosity turbulence models. This work will strictly focus on these types of models. The choice of the turbulent model has a great impact on the computed value of the skin friction coefficient. Therefore, two popular RANS models in the field of CFD have been implemented in CHAMPS to allow their inter-validation. The models implemented are the Spalart-Allmaras one-equation (SA) and the k - ω SST two-equation turbulence models.

3.1.1 CHAMPS software

CHAMPS is an unstructured RANS simulation software [4]. It uses a cell-centered finite volume approach for the convective fluxes and is discretized employing a second-order Roe [54] scheme. The gradients are computed with a Green-Gauss [55] method and are limited with a Venkatakrishnan [56] limiter. The temporal integration is made using an implicit Block Symmetric Gauss-Seidel (SGS) scheme [57]. The turbulence models are solved in a segregated way using the same numerical pseudo-time integration scheme as the flow variables and the turbulent convective fluxes are discretized with a first-order upwind scheme. The droplet trajectories are solved by an Eulerian [33] approach. An iterative Messinger model is employed for the thermodynamic solver [19]. A hyperbolic mesh generation algorithm is used for the geometry evolution [32].

3.1.2 Spalart-Allmaras turbulence model

This turbulence model was proposed by Spalart and Allmaras [37] in 1992. It adds a transport equation for a turbulent variable assembled from empirical results. The model is local and therefore is adapted to all types of mesh. It has already been validated with canonical and airfoil cases with shear flows [37]. The transport equation goes as :

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = P_{\tilde{\nu}} - D_{\tilde{\nu}} + \frac{1}{\sigma} \left[\frac{\partial}{\partial x_j} \left[(\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right] + c_{b2} \frac{\partial \tilde{\nu}}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} \right] \quad (3.1)$$

where ν is the kinematic viscosity, $\tilde{\nu}$ is the turbulence field variable, t is the time variable, x_j is the spatial coordinate in the j direction, u_j is the velocity coordinate in the j direction, d is the wall distance. The other parameters and constants composing the source term are described in Appendix A. Other variations of the model have been implemented in CHAMPS, like the Negative Spalart-Allmaras one-equation model (SA-neg) to address issues with under-resolved grids and non-physical transient states [58].

3.1.3 k - ω SST turbulence model

The principle of the model is to define the turbulence with the kinetic energy of turbulence (k) and the specific dissipation rate (ω). This model was initially formulated by Wilcox [59] to improve the accuracy for wall-bounded flows and flows with high-pressure gradients. Unfortunately, this model is highly dependent on the boundary conditions and turbulence values. Menter fixed the problem, using only the k - ω model near the wall [60], creating the k - ω SST turbulence model. The model is defined as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] \quad (3.2)$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\gamma}{\nu_t} P - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho \sigma_{\omega 2}}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (3.3)$$

where t is the time variable, x_j is the spatial coordinate in the j direction, u_j is the velocity coordinate in the j direction, ρ the air density and P a source term. The remaining constants and functions are defined in Appendix A. Variants have been implemented in CHAMPS, such as the k - ω SST-V(m) [61], to redefine the computation of the vorticity and limiters for the production term P . The k - ω SST-2003(m) [62] variants modify the computation of the eddy viscosity to use the strain invariant for the vorticity and change some limiters of the model. The k - ω SST-2003 model is used with the transition extension of Section 3.4.

3.2 Verification of the turbulence models

The Langley Research Center (LRC) proposes a database of well-established cases [63] to verify that models are implemented correctly. The site also helps to understand and compare the predictions of a variety of models on fundamental flow problems in the validation database. A common verification case for both the SA model and the $k-\omega$ SST model is the two-dimensional zero pressure gradient Flat Plate case. Because the purpose here is primarily verification, the experiment is not specifically looked at. The case parameters are a Mach of 0.2, a Reynolds number of 10 million and a reference length of 2 meters. The height of the grid is half the plate length. A farfield condition is imposed at the top, while inlet and outlet boundaries are imposed on the sides. The reference temperature, T_{ref} , is of 300 K. While the outlet pressure and temperature correspond to the reference values, a total temperature of $1.008T_{ref}$ and a total pressure of $1.0283P_{ref}$ are imposed at the inlet. Figure 3.1 shows the grid convergence of the drag coefficient and the turbulent eddy viscosity profile at $x = 0.97$ m in comparison with other RANS codes: CFL3D [64] and FUN3D [65]. The results have been produced by Parenteau *et al.* [4].

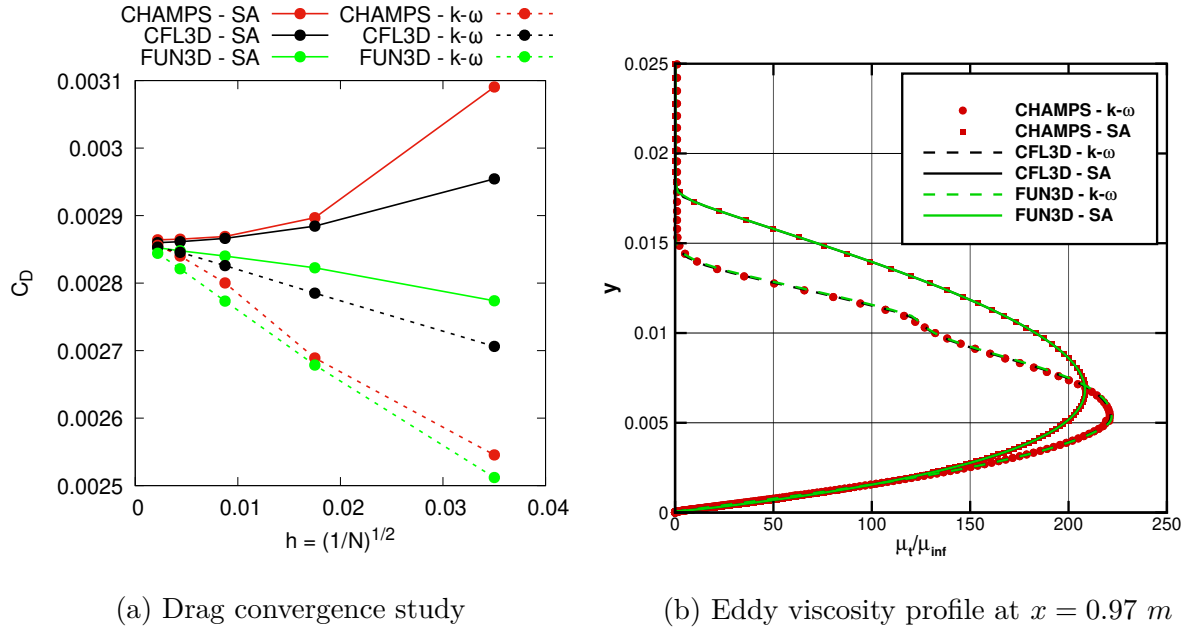


Figure 3.1 Verification of $k-\omega$ SST and SA turbulence models on the LRC Flat Plate case ($Ma = 0.20$, $Re = 10$ million) [4]

In Figure 3.1a, it can be observed that the order of convergence of both models conforms with the two compressible RANS codes used by the National Aeronautics and Space Administra-

tion (NASA). CFL3D is a cell-centered structured-grid code, and FUN3D is a vertex-centered unstructured-grid code. Both codes use Roe's Flux Difference Splitting and a UMUSCL upwind approach. The turbulent eddy viscosity profile is extracted at the location $x = 0.97$ m. With both models, CHAMPS, CFL3D and FUN3D converge toward the same value for the drag coefficient as the grid is refined. For the eddy viscosity profile in Figure 3.1b, the results are one on top of the other. The field values of the turbulent variable k and ω were also compared and are matching CFL3D and FUN3D results.

Additionally, the local values of the skin friction are analyzed. The results are shown in Figure 3.2. The local skin friction values are matching for the three codes. Complementary to Figure 3.1, Figure 3.2 verifies the turbulence models used in CHAMPS. Similar results are obtained with the variants of the models. The validation of the models has already been done by their authors. However, Chapter 4, will compare the results of these models with experimental data, when a roughness correction is applied at the wall.

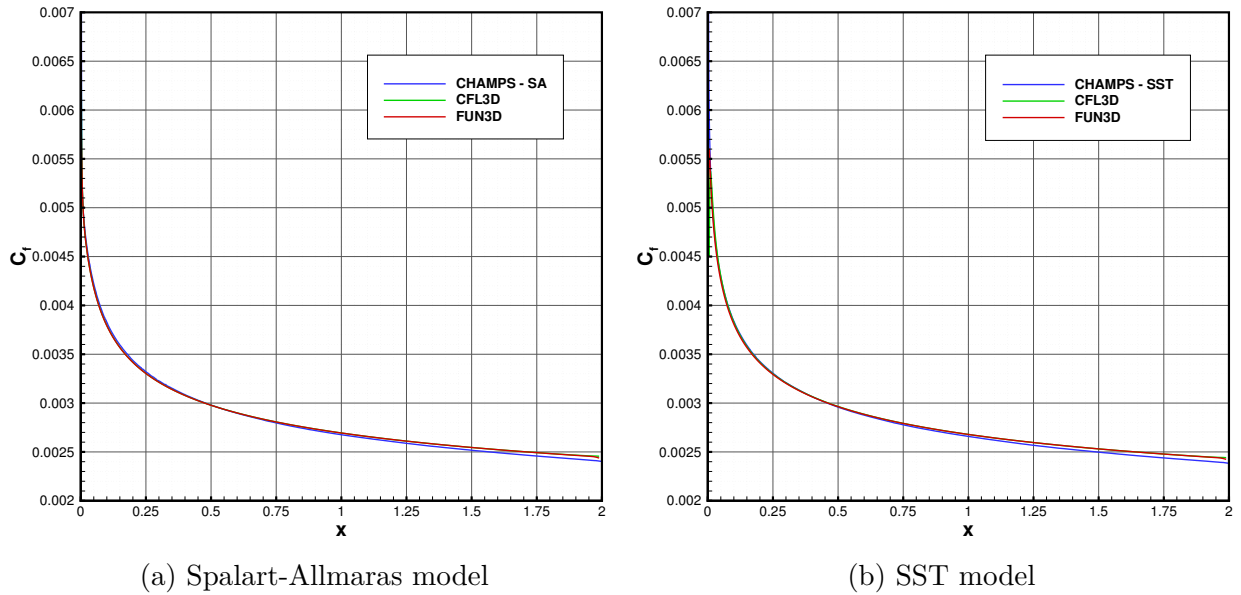


Figure 3.2 Local skin friction of k - ω SST and SA turbulence models on the LRC Flat Plate case ($Ma = 0.20$, $Re = 5$ million, grid 545×385)

3.3 Evaluation of the heat transfer coefficient

Since the evaluation of the heat transfer coefficient is strongly dependent on the flow computation, the previously proposed turbulence models are used in CHAMPS. The main effect of the turbulence model is to compute the adequate value of the turbulent friction coefficient. This effect is transposed into the heat transfer computation since the turbulent eddies also

raise the heat transfer. Using the mean energy equation, the convective heat transfer can be written as:

$$q_{t,j} = -k_c \frac{\partial T}{\partial x_j} \quad (3.4)$$

with $k_c = \alpha_t \rho c_p$, α_t being the turbulent thermal diffusivity. The temperature gradient is computed from the flow solution. Several thermal models are available to compute the thermal diffusivity, but they do not improve significantly the accuracy of the prediction [66]. In CHAMPS, the heat transfer at the wall is defined as:

$$\dot{Q}_{wall} = c_p \left(\frac{\mu_l}{Pr} + \frac{\mu_t}{Pr_t} \right) \frac{\partial T}{\partial \vec{n}} \Big|_{wall} \quad (3.5)$$

where the term $\partial T / \partial \vec{n}$ is determined using the temperature gradient. The ratio of momentum diffusivity to thermal diffusivity varies in the viscous sublayer. The values are normally assumed to be $Pr_t = 0.9$, which is the value in the logarithmic region [67] and $Pr = 0.707$ for CFD codes. However, the use of this assumption may not be as accurate in the presence of pressure gradients, high freestream turbulence levels and rough walls. The HTC is computed using the recovery temperature, since viscous dissipation cannot be neglected, and the isothermal user-imposed wall temperature:

$$HTC = \frac{\dot{Q}_{wall}}{T_{wall} - T_{rec}} \quad (3.6)$$

A different convective heat flux is used in the thermodynamic balance determining ice accretion. Its value is obtained employing the calculated ice surface temperature determined by the thermodynamic model, which differs from the imposed wall temperature:

$$\dot{Q}_{conv} = \frac{HTC}{T_{surf,ice} - T_{rec}} \quad (3.7)$$

The turbulence or transitional models impact the value of the shear stress by the turbulent eddy viscosity μ_t , therefore modifying the heat transfer at the wall. Since heat transfer is strongly dependent on the definition of the boundary layer, considering only a turbulent boundary layer may not be enough. The current method of calculating μ_t leads to an overestimation of the heat transfer in regions where the boundary layer is laminar. To compensate for this problem, additional equations have been added to trigger or not the turbulent model depending on the flow regime. The methods for the flow computation must be modified to:

1. Predict the position of the laminar-turbulent transition of the boundary layer;

2. Calculate the value of the shear stress for a laminar-turbulent boundary layer.

Transitional models are good candidates since they can be implemented in addition to the turbulence models for RANS codes. Other methods, like the e^n method, are available for two-dimensional boundary layer codes, based on linear stability theory [68]. However, this method solves non-local variables that require the integration of the boundary layer, which is very impractical and can show convergence problems when coupled with RANS codes [69]. Thus, the implementation of transitional models is chosen for CHAMPS. The description and implementation of these equations are presented in the next section, for the SA and $k-\omega$ SST2003 models.

3.4 Transition extension for turbulence models

The $\gamma-\tilde{Re}_{\theta t}$ transition extension developed by Langtry and Menter [70] was originally coupled with the $k-\omega$ SST2003 turbulence model. Later it was coupled with the SA model in the work of Medina and Baeder [71]. The model uses the intermittency (γ) to control the production of turbulence in the boundary layer and the transition momentum thickness Reynolds number ($\tilde{Re}_{\theta t}$) to trigger the intermittency. The local flow is fully turbulent when $\gamma = 1$ and fully laminar when $\gamma = 0$. The two equations are the following [72]:

$$\frac{\partial(\rho\gamma)}{\partial t} + \frac{\partial(\rho u_j \gamma)}{\partial x_j} = P_\gamma - E_\gamma + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_f} \right) \frac{\partial \gamma}{\partial x_j} \right] \quad (3.8)$$

$$\frac{\partial(\rho \tilde{Re}_{\theta t})}{\partial t} + \frac{\partial(\rho u_j \tilde{Re}_{\theta t})}{\partial x_j} = P_{\theta t} + \frac{\partial}{\partial x_j} \left[\sigma_{\theta t} (\mu + \mu_t) \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} \right] \quad (3.9)$$

The source terms and the other constants are explained in Appendix A and in [70,72]. There are slight differences when the coupling is done with the $k-\omega$ SST2003 or the SA turbulence model. Note that the turbulence intensity with the $k-\omega$ SST2003- $\gamma-\tilde{Re}_{\theta t}$ model is computed from :

$$Tu = 100 \frac{\sqrt{2k/3}}{U} \quad (3.10)$$

when it is considered constant for the SA- $\gamma-\tilde{Re}_{\theta t}$ model.

3.4.1 Verification and validation of the models

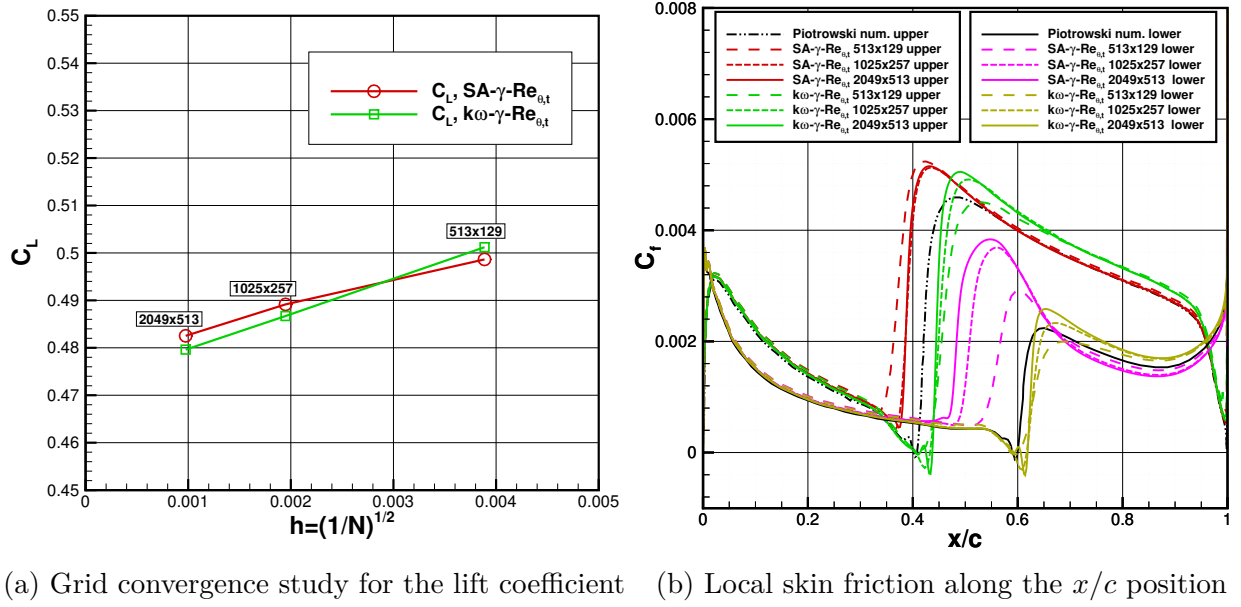
Multiple test cases with experimental results are available to validate the transitional models. However, the LRC has not yet published verification test cases for these models. In this work,

an experiment on the NLF0416 airfoil, which was designed for natural laminar flows, is used for the validation of the models with Somers [73] experiments. This experiment was done in the Low Turbulence Pressure Tunnel (LTPT) located at the LRC.

The flow conditions are a Reynolds number of 4.0 million and a Mach number of 0.1. The choice of turbulence intensity in the field is a problem with the transitional models. Normally, this parameter can be measured in wind tunnels, but in this case, it is unknown. A result from a simulation at a specific turbulence intensity will almost never fall on the measured value at the same turbulence intensity. Therefore, the models normally need to be tweaked for a specific case and the experimental value is only employed to know the amplitude of the turbulent intensity that needs to be used. For this case, the value of 0.15% is utilized for both models to be consistent with the value chosen by Piotrowski and Zingg [74], which is the numerical reference. This is also the recommended value by the Transition Modelling and Predictive Capabilities Seminar (TCMPS) guidelines [75]. The transition mechanism is typically a natural transition for the upper side and a separation-induced transition for the lower side because of a small laminar separation bubble that appears for positive Angles of Attack (AoA).

Grid convergence studies for the SA- γ - $\tilde{Re}_{\theta t}$ and the k - ω - γ - $\tilde{Re}_{\theta t}$ models are conducted with meshes of size 513×129 , 1025×257 and 2049×513 . The results are displayed in Figure 3.3. The lift coefficient is more sensitive to the grid resolution than the drag coefficient. For the transition location, Figure 3.3b shows that mesh independency is reached, except on the lower side for the results obtained with the SA- γ - $\tilde{Re}_{\theta t}$ model. This difference could be explained by comparing the transition types of the two models. At $C_L \approx 0.5$, Figure 3.4 shows a natural transition on the lower side for the SA- γ - $\tilde{Re}_{\theta t}$ model, but a separation-induced transition for the k - ω - γ - $\tilde{Re}_{\theta t}$ model caused by a separation bubble. The SA turbulence model is expected to be less accurate than the k - ω turbulence model for predicting shear flows and separated flows. The natural transition mechanism is more sensitive to grid resolution.

Figure 3.4 shows that the transition locations are in agreement with the experimental data. This agreement becomes better on the lower side as the transition mechanism switches from a natural to a separation-induced transition for $C_L > 0.5$ because of the presence of a laminar separation bubble. The separation bubbles are close to the experimental natural transition locations and are less impacted by the changes in turbulence intensity. It may explain why the two models have similar transition locations with the same freestream turbulence intensity while they often need to be adjusted separately. Other results are present in [5]. The transition locations are computed using the maximum of the derivative of the friction coefficient according to x .



(a) Grid convergence study for the lift coefficient (b) Local skin friction along the x/c position

Figure 3.3 Grid convergence study for the NLF0416 case ($Ma = 0.10$, $Re = 4$ million, $Tu = 0.15\%$, $AoA = 0.0^\circ$) [5]

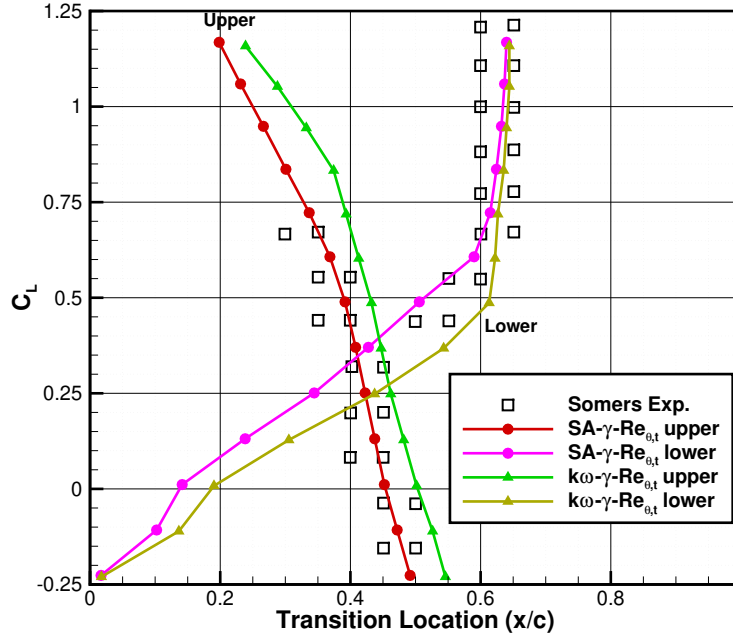


Figure 3.4 Lift coefficient (C_L) as a function of the transition location for the NLF0416 case ($Ma = 0.10$, $Re = 4 \times 10^6$, $Tu = 0.15\%$, $grid = 1025 \times 257$) [5]

3.4.2 Problems of turbulence/transitional models for the HTC computation

To compute the correct tendency of the ice shapes, the HTC must be computed in accordance with experimental data obtained on typical airfoil cases. During the ice accretion process, roughness grows on the surface, controls the development of the boundary layer and affects the convective heat transfer. Multiple models have been developed to modify the boundary conditions and source terms of the turbulence models to consider the effect of the surface roughness. These models, accompanied by ice shape results, will be presented in Chapter 4.

3.5 Conclusion

In this chapter, turbulence models implemented in CHAMPS are presented and verified. Since the heat transfer coefficient is influenced by the flow regime, the transition of the flow for lower Reynolds numbers is considered with an extension for the current turbulence models. The models are verified and validated. However, to improve the accuracy of the predicted heat transfer, a roughness model needs to be coupled with the turbulence/transitional models.

CHAPTER 4 ROUGHNESS EXTENSIONS FOR TURBULENCE MODELS

This chapter suggests an equivalent sand grain approach to include the roughness in the turbulence/transitional models. The limitations of such methods are presented, as well as the distinct extensions for the SA and the $k\text{-}\omega$ SST models. These formulations are validated with the Mills and Hang [76] skin friction correlation on a Flat Plate and verified by comparing the heat transfer on an airfoil case with a well-verified code while varying the roughness. To consider the shift of the transition location due to roughness, an additional equation is implemented to transport the effect of the roughness. This implementation is also validated with a Flat Plate case. The impacts of the different models present in this chapter are assessed with the generation of ice shapes associated with the NASA Lewis Icing Research Tunnel (IRT) airfoil cases. For these cases, the effect of the number of layers and the turbulent intensity is also studied.

4.1 Equivalent sand grain approach

Different approaches can be used to compute a roughness in RANS codes. Roughness can be classified into two types. The d-type (1) is composed of grooves in the smooth surface and the k-type (2) is composed of protuberances on the surface [77]. This work will focus on the k-type roughness. A method employed to compute the roughness called the *discrete element approach* adds a roughness by an extra term in the flow equations to account for the obstacle it creates on the flow as well as the heat flux and the drag it causes. Unfortunately, this requires complex changes in the flow equations and the practical applications for such a model are not well-established in the scientific community. Another approach is to use an *equivalent sand grain* which does the parallel between the exact roughness of the geometry and the roughness given as an input of the model. The height of the real roughness is converted with an empirical correlation [78] to an equivalent sand grain height, as used in Nikuradse's [36] experiments. In the models, the roughness enhances the turbulent eddy viscosity near the wall, which increases the skin friction as well as the heat flux. Note that the calibration is based on skin-friction values, thus leaving the heat flux uncalibrated. Since these models are well documented and apply to the turbulent models present in CHAMPS, they have been implemented to simulate the effect of the roughness. With these models, the eddy viscosity can either be null or finite at the wall boundary, depending on whether the wall is at the bottom of the roughness or part-way as shown in Figure 4.1.

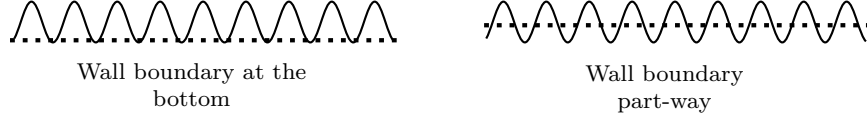


Figure 4.1 Wall boundary possible locations when the wall is rough

The choice of the approach depends on the size of the roughness. Since Nikuradse [36] provided relations between the shift of the velocity profile and the equivalent sand grain roughness, these results have been used in the last years to establish roughness correlations. A non-dimensional variable employed to define the roughness is:

$$k_s^+ = u_\tau \cdot \frac{k_s}{\nu} \quad (4.1)$$

where k_s is the equivalent sand grain height, ν is the fluid kinematic viscosity and $u_\tau = \sqrt{\tau_{wall}/\rho_{wall}}$, τ_{wall} being the shear stress at the wall and ρ_{wall} the air density at the wall. This variable defines the roughness properties. Different categories of roughness exist [36]:

1. Hydraulically smooth ($k_s^+ < 5$): The roughness has no impact on the skin friction and the surface is considered smooth. The viscosity damps the effect of the roughness which is within the viscous sub-layer;
2. Transitionally rough ($5 < k_s^+ < 70$): The roughness decreases the height of the viscous sub-layer and increases the skin friction. The roughness size and distribution pattern have an impact on skin friction;
3. Fully rough ($k_s^+ > 70$): The skin friction is independent of the viscous forces and the viscous sub-layer is destroyed.

A majority of the roughness extensions are applicable for fully rough cases since the effects of the roughness on the skin friction in this regime are well-defined. However, k_s^+ varies along a surface and transitionally rough regions can be encountered.

4.2 Extensions for classical turbulence models

To have a physical value for the heat transfer coefficient depending on the surface roughness, extensions are added to both turbulence models available in CHAMPS. For these models, several hypotheses are used as a premise:

1. The roughness-element size in any direction is small compared to the boundary-layer thickness;
2. The boundary of the computational domain is smooth;
3. The velocity wall boundary condition is zero.

4.2.1 Spalart-Allmaras roughness extension

Two methods were initially proposed independently by Boeing and ONERA to take into account the wall roughness with the Spalart-Allmaras model. Both have an impact on the wall boundary condition of the turbulent variable. They were summarized by Aupoix and Spalart [78] and suggested as viable roughness extensions. For the ONERA method, a non-zero Dirichlet condition is imposed for the modified eddy viscosity at the wall. For the Boeing method, a Neumann condition is imposed at the wall. Since convergence problems are present with the ONERA method, the Boeing extension is employed for this work. The wall distance is employed in the Spalart-Allmaras model, this one is shifted by a value function of the equivalent sand grain roughness. The new wall distance, d_{new} , is defined as:

$$d_{new} = d_{smooth} + d_{rough} \quad (4.2)$$

where d_{smooth} is the physical wall distance used when no roughness is present and d_{rough} is the shift of the wall distance. The value for d_{rough} normally employed is $0.03k_s$. The damping function of the model is modified to increase the accuracy in transitionally rough regimes:

$$\chi = \frac{\tilde{\nu}}{\nu} + 0.5 \frac{k_s}{d_{new}} \quad (4.3)$$

The boundary condition employed is defined by:

$$\frac{\partial \tilde{\nu}}{\partial n} = \frac{\tilde{\nu}}{d_{new}} \quad (4.4)$$

where n is the normal to the wall. The Boeing model is used to change the boundary condition at the wall of the transported quantity in the SA model, based on a modified wall distance function of the roughness. This model also requires a modification of the source terms in the flow field.

4.2.2 k - ω SST roughness extension

For the k - ω SST model, no extension formulation was present in CHAMPS. Multiple extensions are suggested in the literature. The first one was proposed by Wilcox [79], but unfortunately, it creates interferences with the SST limiter, limiting the iterative convergence of the solution. Some correlations were also proposed by Hellsten *et al.* [80] and by Knopp *et al.* [81]. The main goal of these correlations is to intensify the turbulence at the wall through the turbulent kinetic energy and the specific turbulence dissipation rate equations. Thus, the simplicity of these models resides in the fact that they only change the model boundary conditions at the wall because the conditions in the logarithmic region have little influence on the solution. The problem with Wilcox's [79] correction is that it is using a noncontinuous function at the wall which causes difficulties for the convergence and unrealistic behaviors. While Hellsten *et al.* [80] fixed this problem, their correlation is not applicable for large values of roughness. Knopp *et al.* [81] strongly underestimate the velocity shift in the transitionally rough regime. These correlations are therefore not applicable in CHAMPS. The correlation proposed by Aupoix [82], based on Colebrook and White [83] results has been implemented in CHAMPS in a non-dimensional form:

$$k_{wall}^+ = \max(k_0^+) \quad (4.5)$$

$$k_0^+ = \frac{1}{\sqrt{\beta^*}} \tanh \left[\left(\frac{\ln(k_s^+/30)}{\ln(10)} + 1 - \tanh(k_s^+/125) \right) \tanh(k_s^+/125) \right] \quad (4.6)$$

$$\omega_{wall}^+ = \frac{300}{k_s^{+2}} (\tanh(15/(4k_s^+)))^{-1} + \frac{191}{k_s^+} (1 - \exp(-k_s^+/250)) \quad (4.7)$$

4.3 Validation of equivalent sand grain roughness models

In this section, the models implemented are validated on a typical Flat Plate case with a global value for the roughness. To do so, the skin friction amplification based on the roughness is validated using the Mills and Hang [76] correlation. Then, the computation of the heat transfer coefficient is verified by comparing the values with NSCODE [19] and LEWICE 2.0 [15].

4.3.1 Roughness - Flat Plate case

To validate both turbulence models with rough wall extensions, the empirical correlation by Mills and Hang [76] is employed. They added the wake profile to the logarithmic velocity profile for rough walls and numerically integrated it to obtain the value of the skin friction coefficient for rough walls. For a fully rough plate ($k_s^+ > 70$), Mills and Hang [76] give the correlation:

$$C_f = \left[3.476 + 0.707 \ln \left(\frac{x}{k_s} \right) \right]^{-2.46} \quad (4.8)$$

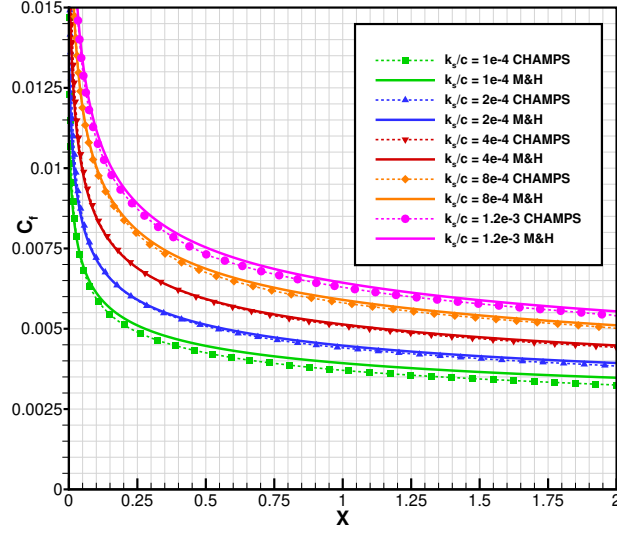
where k_s is the equivalent sand grain roughness height. The case is a zero pressure gradient Flat Plate with an AoA of 0° . The length of the plate is 2 *m* with a 0.25 *m* entry zone. The height of the domain is also 2 *m*. The y^+ value is inferior to 0.1 which is recommended for roughened surfaces. The grid used has 545 nodes along the plate and 385 nodes toward the farfield. The Reynolds number based on the length of the plate is 4 million and the Mach number is 0.2.

For the boundary conditions, two types are investigated. The first type combines a subsonic inlet with a specified total pressure ratio $P_{tot}/P_\infty = 1.0283$ and total temperature ratio $T_{tot}/T_\infty = 1.008$ as defined for the zero pressure case of the LRC [63]. The outlet is subsonic with a specified total pressure ratio P_{tot}/P_∞ and total temperature ratio T_{tot}/T_∞ of one. The second type of boundary conditions uses farfield conditions at the inlet and outlet of the domain. For all the simulations, a farfield boundary condition is employed at the top of the domain, a viscous wall boundary condition is used for the Flat Plate and a symmetry condition is employed in the buffer zone.

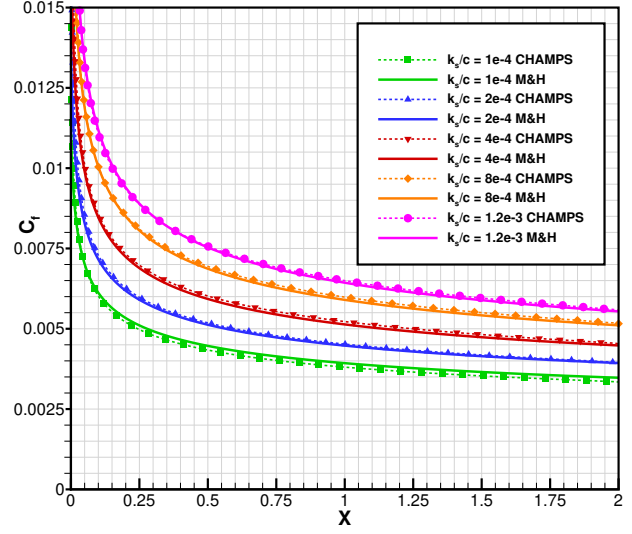
Figure 4.2 shows the friction coefficient along the position on the Flat Plate for multiple values of the equivalent sand grain roughness normalized by the plate length. The values are $k_s/c = [1, 2, 4, 8, 12] \times 10^{-4}$, defining a range of roughness normally observed in icing applications. Slightly better results are achieved with the farfield condition at the inlet and at the outlet. The flow density residuals are reduced by ten orders of magnitude. The skin friction follows the Mills and Hang [76] relation for the SA model, but minor differences appear at higher roughness values for the $k-\omega$ SST model. These differences are in line with other results from the literature. The lower values of k_s are in the transitionally rough regime.

4.3.2 Heat transfer - Airfoil case

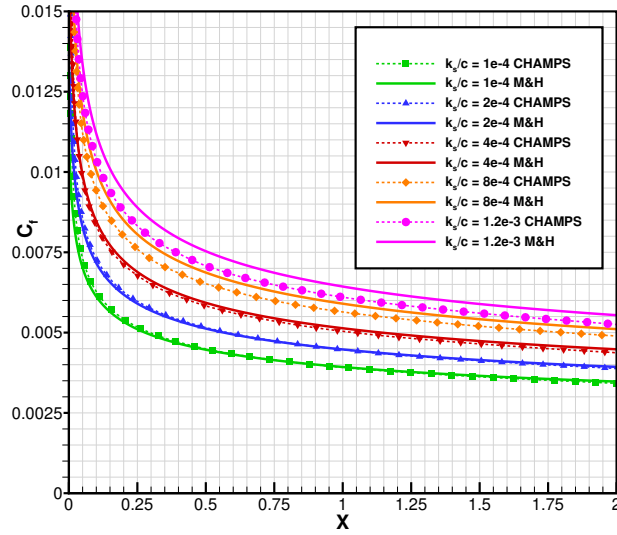
In this section, the heat transfer on the rough surface is verified on airfoil cases. To do so, the numerical data available from LEWICE 2.0 [15] on NASA IRT cases [2] have been used



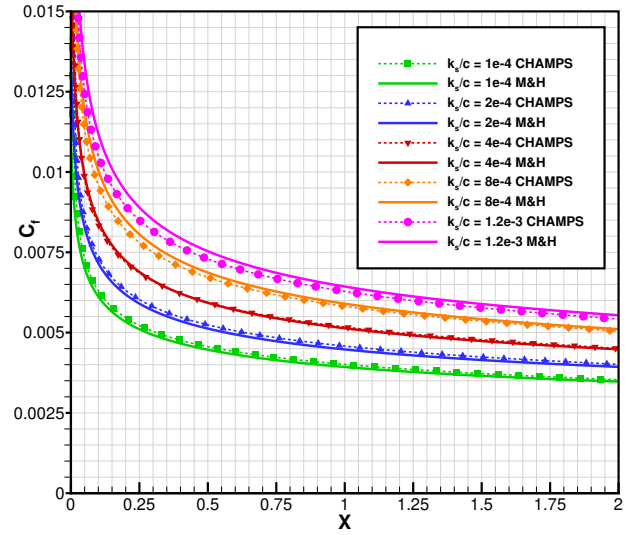
(a) SA - Subsonic inlet/outlet



(b) SA - Farfield



(c) SST - Subsonic inlet/outlet



(d) SST - Farfield

Figure 4.2 C_f vs x , Flat Plate comparison with Mills and Hang (*M&H*) correlation for varying roughnesses ($Ma = 0.20$, $Re = 4$ million, $L = 2$ m)

for the comparison, as well as the results from NSCODE-ICE [84], the previous icing solver utilized at Polytechnique Montreal. Cases 421 and 425 are employed for the comparison, since they correspond respectively to a rime-type case and a glaze-type case, covering the two major icing categories studied by the icing community. The parameters of the cases are displayed in Table 4.1. The roughness formulations for SA and $k-\omega$ SST models are employed in CHAMPS with a grid of 385 nodes in the tangential direction and 257 nodes in the normal direction. The results of the heat transfer coefficient on the rough airfoil along the curvilinear distance from the leading edge are presented in Figure 4.3. The flow residuals are reduced by 10 orders of magnitude. The results are in good agreement with the numerical results of NSCODE-ICE [84] and LEWICE 2.0 [15]. Good practice suggests that a y^+ inferior to 0.1 must be used when a rough wall formulation is employed. For these cases, a y^+ slightly inferior to 1 is giving similar results, so this mesh is employed for the next simulations to reduce the computation costs.

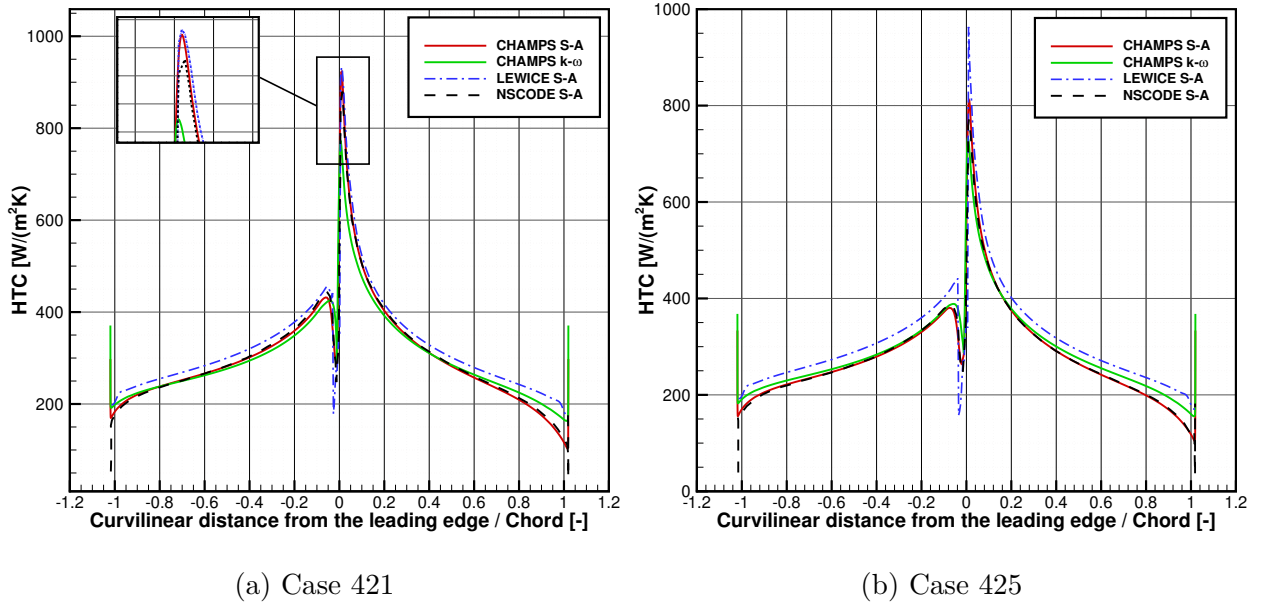


Figure 4.3 Verification of the HTC vs s for NASA IRT cases 421 and 425 compared to LEWICE 2.0 and NSCODE numerical data ($U = 67.1\text{m/s}$, $\text{MVD} = 20\text{ }\mu\text{m}$)

The results show good agreement with NSCODE-ICE [84], which is using the SA model with the Boeing roughness extension. The same equivalent sand grain roughness height values used by NSCODE-ICE [84] and LEWICE 2.0 [15] are employed for the computations. The values are $k_s = 701.6\text{ }\mu\text{m}$ for case 421 and $k_s = 335.4\text{ }\mu\text{m}$ for case 425. The computation of the heat transfer coefficient of CHAMPS and NSCODE-ICE [84] requires an imposed temperature at the wall. The value employed is $T_{wall} = 1.05T_\infty$ for both codes. This value is generally the

better compromise to calculate the heat transfer coefficient since it should not be too close to the recovery temperature and not too far. The recovery temperatures, which are within 0.4% of the fixed wall temperatures, are respectively 270 K and 246 K for cases 421 and 425. With the SA turbulence model, the curves are practically on top of NSCODE-ICE [84] results, using the same mesh. The peak of the HTC is higher with CHAMPS using the SA model compared to the k - ω SST model in Figure 4.3a. Near the trailing edge, the CHAMPS k - ω SST solutions differ from the SA solutions and are closer to LEWICE 2.0 [15] solutions. The important region for icing applications is near the leading edge. It is possible to observe that the value at the stagnation point, at $s \approx -0.04$, is overestimated by CHAMPS and NSCODE-ICE [84] compared to LEWICE 2.0 [15].

4.4 Roughness transport equation for transitional models

The problem with the roughness extensions of Section 4.2 becomes apparent when trying to apply them in combination with the transitional equations. With these extensions, the effect of the roughness on the skin friction shift is observed, but another property of the roughness is not taken into account. This property is the upstream displacement of the laminar/turbulent transition when roughness is applied. The amplitude of the turbulent heat transfer can be captured with the rough wall boundary conditions previously discussed. To predict glazed ice shapes, it is important to determine if the boundary layer is laminar or turbulent. One can assume that the roughness of the ice triggers the transition to a turbulent boundary layer. However, Habashi [85] noted the importance of including the laminar-transition effect to improve icing simulation by capturing the lower horn in cases with a positive angle of attack. The effect of the transient heat transfer on ice has been observed by Han and Palacios [86] with airfoil cases from the NASA IRT. Few numerical models of roughness-induced transition have been developed. These models, coupled with rough wall boundary conditions, permit a more accurate assessment of the impact of roughness on heat transfer. For higher Reynolds numbers, the transition is close to the leading edge, the transition computation is not necessary for the simulation accuracy. However, according to experimental research [86], roughness-induced transition affects the shape of ice for low Reynolds numbers. A way to capture the transition onset is to use the transport equation for the *Roughness Amplification* variable proposed by Dassler *et al.* [87] and extended by Langel *et al.* [88] for airfoil cases.

4.4.1 Model formulation

The roughness shifts the laminar-turbulent transition upstream in the flow, which can be perceived in the local skin friction values. The transition location is also influenced by other effects like the turbulence intensity, the pressure gradient and the Reynolds number [88]. The roughness extensions that have been implemented do not predict the right position of the transition due to the roughness effect. The model proposed by Dassler *et al.* [87] and modified by Langel *et al.* [88], is based on the transitional model from Langtry and Menter [70] and uses the intermittency concept to trigger the transition. The advantage of this model is that it is based on local values. A transport equation is added and employs a new variable called the *Roughness Amplification*. The *Roughness Amplification* transport equation is:

$$\frac{\partial (\rho A_r)}{\partial t} + \frac{\partial (u_j A_r)}{\partial x_j} = \frac{\partial}{\partial x_j} \left[\sigma_{Ar} (\mu + \mu_t) \frac{\partial A_r}{\partial x_j} \right] \quad (4.9)$$

where A_r is the *Roughness Amplification* variable and $\sigma_{Ar} = 10.0$ is a model constant. The rough wall boundary is defined as:

$$A_r|_{wall} = c_{Ar1} k_s^+ \quad (4.10)$$

where $c_{Ar1} = 8.0$. The transport equation allows to diffuse and convect the effect of the roughness in the flow field. It also considers the flow history effects since there is a lag between the roughness position and where the boundary layer reacts to this roughness. Initially, the model had a source term P_{Ar} that amplified the value A_r near the wall. Further revisions of the model removed this source term and arrived at the same results by amplifying the effect of A_r near the wall. Eq. (4.9) is coupled to the RANS equations by the production term of the $\tilde{Re}_{\theta t}$ equation. This production term changes from:

$$P_{\theta t} = \frac{\rho}{T} c_{\theta t} (Re_{\theta t} - \tilde{Re}_{\theta t}) (1 - F_\theta) \quad (4.11)$$

with $T = 500\mu/(\rho U^2)$, a time scale here for dimensional reasons, to:

$$P_{\theta t} = \frac{\rho}{T} [c_{\theta t} (Re_{\theta t} - \tilde{Re}_{\theta t}) (1 - F_\theta) - b F_{Ar}] \quad (4.12)$$

The new term F_{Ar} is function of A_r . In its new form, F_{Ar} is cubic for low A_r values and linear at higher values. It is also multiplied by a factor b for lower values of $\tilde{Re}_{\theta t}$. When $\tilde{Re}_{\theta t}$ reaches its minimum value, b is set to 0 and is close to one when $\tilde{Re}_{\theta t}$ is high. When

no roughness is amplified, the RANS equations are unchanged. For F_{Ar} , Langel *et al.* [88] proposed:

$$F_{Ar} = \begin{cases} c_{Ar2} A_r^3 & \text{if } A_r < C_{Ar}, \\ c_{Ar3}(A_r - C_{Ar}) + c_{Ar2} C_{Ar}^3 & \text{if } A_r \geq C_{Ar} \end{cases} \quad (4.13)$$

with $c_{Ar2} = 0.0005$, $c_{Ar3} = 2.0$ and $C_{Ar} = (c_{Ar3}/(3 \cdot c_{Ar2}))^{0.5}$. The blending function b is used when the local value of $\tilde{Re}_{\theta t}$ is near the prescribed minimum of the transitional model to no longer decrease the production term. The function is sinusoidal to insert this effect gradually:

$$b = \left[\frac{1}{2} \sin \left(\frac{\pi}{155} \tilde{Re}_{\theta t} - \frac{97\pi}{155} \right) + \frac{1}{2} \right]^2 \quad (4.14)$$

Therefore, this function attains its peak when $\tilde{Re}_{\theta t} = 180$. However, in conventional cases, $\tilde{Re}_{\theta t}$ can be over 1000. Periods of b are then observed in the field and the production term is deactivated when it should be activated, changing the solution and affecting the residual convergence of Eq. (4.9). To fix this problem, the function is only activated when the value of $\tilde{Re}_{\theta t}$ is under 180. When $\tilde{Re}_{\theta t}$ is higher than 180, the value of b is fixed to 1. The advantage of the model from Langel *et al.* [88] for the application in CHAMPS is the fact that it is built on top of the transitional models and roughness extensions in CHAMPS in the form of a fifth turbulence equation for the k - ω SST2003- γ - $\tilde{Re}_{\theta t}$ model, and a fourth for the SA- γ - $\tilde{Re}_{\theta t}$ model. The same equation can be applied to both models.

4.5 Verification and validation of the model

The roughness extension proposed by Dassler *et al.* [87] and Langel *et al.* [88] was originally calibrated on Feindt's [89] experimental results for a Flat Plate case. The model was firstly verified when coupled with the k - ω SST2003- γ - $\tilde{Re}_{\theta t}$ model and the rough wall boundary conditions proposed by Wilcox [79]. In this work, the SA turbulence model coupled with the γ - $\tilde{Re}_{\theta t}$ transition extension and the Boeing rough wall boundary condition [78] is employed instead. This choice is made since this model is more stable, shows increased iterative convergence, estimates more accurately the shift of the friction coefficient and does not need parameters like the freestream ratio μ_t/μ and the turbulence decay to be specified by the user. Therefore, this combination of models is verified here. For this case, the roughness is characterized by its equivalent sand grain height. A mesh of 0.2 meter height containing a 0.2 meter Flat Plate is used with an entry region of 20% of the length of the plate. A speed at the entry of 100 m/s is set to match the Reynolds number of the experiment, which is 1.33 million. The Mach number is 0.3. Farfield conditions are imposed at the inlet, the

outlet and the upper wall of the mesh. For numerical results from Langel *et al.* [88], a no-slip upper wall boundary is employed at a distance of 14.95% of the length of the plate to fix the pressure gradient and simulate the experimental conditions. The freestream turbulence intensity is set to 1.02% to match the transition position when no roughness is applied. The prescribed value is 1.1% for the experiment [89]. This is close to the value of 0.91% utilized by Dassler *et al.* [87] and Langel *et al.* [88]. The contrast of the values could be due to the use of different boundary conditions and turbulence models. Figure 4.4 shows the effect of the global roughness value on the transition location on the Flat Plate. The results are compared to numerical results from Langel *et al.* [88] and Feindt's [89] experiment. To do the comparison, the roughness Reynolds number, Re_{ks} , is used. This one is defined by:

$$Re_{ks} = \frac{U_k k_s}{\nu} \quad (4.15)$$

where U_k is the velocity in an undisturbed boundary layer at height k_s and ν is the kinematic viscosity of the air set to $14.96 \times 10^{-6} \text{ m}^2/\text{s}$.

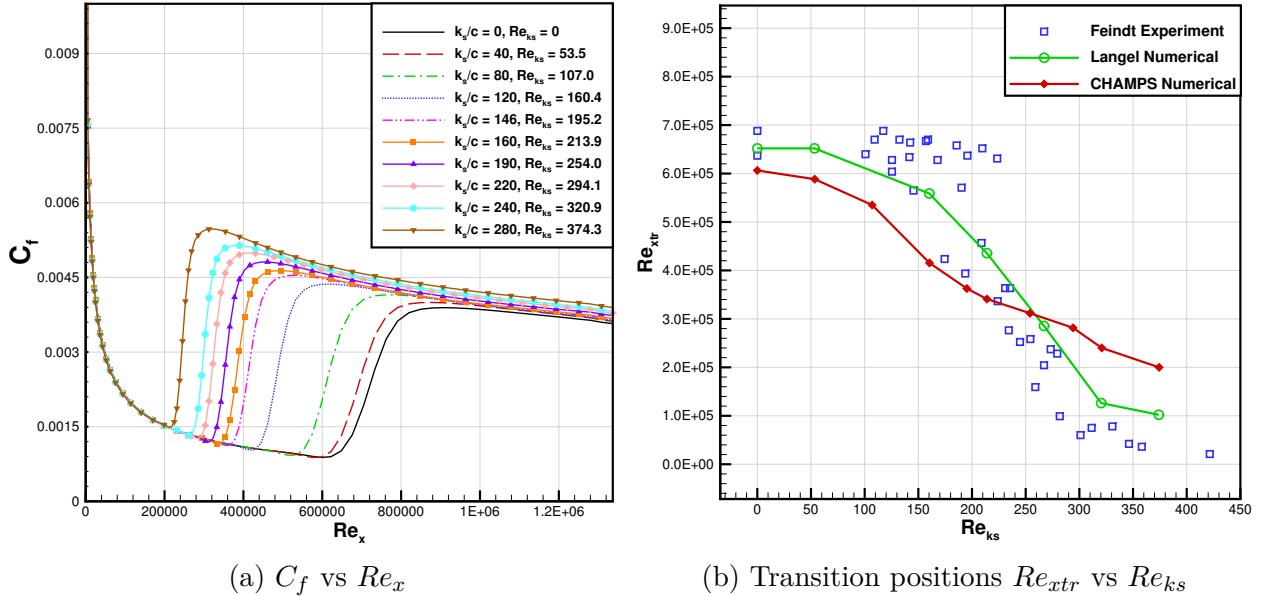


Figure 4.4 Verification and validation of the *Roughness Amplification* equation with the SA- γ - $\tilde{Re}_{\theta t}$ model for the zero pressure gradient Flat Plate with varying sand grain roughnesses ($AoA = 0^\circ$, $Mach = 0.1$, $Tu = 1.02\%$, $Re = 1.33$ million)

In Figure 4.4a, a translation of the friction coefficient in the turbulent region is caused by the rough wall boundary condition while increasing the nondimensional sand grain roughness. The *Roughness Amplification* equation causes the upstream shift of the transition onset when

increasing roughness. As in the experiment, the streamwise location of the minimum friction coefficient is used to determine the transition location. Another choice for the transition location criterion may affect the results. In Figure 4.4b, Re_{xtr} represents the local Reynolds number where the transition occurs. The differences in the transition locations compared to experimental and numerical results can be due to the use of the SA- γ - $\tilde{Re}_{\theta t}$ transitional model instead of the k - ω SST2003- γ - $\tilde{Re}_{\theta t}$ transitional model. The choice of the freestream turbulence intensity can also have an impact. Overall, the results are judged acceptable for this work, since transition position shifts and overall trends are captured. Furthermore, the effect of the pressure gradient on transition locations has been validated by Langel *et al.* [88].

4.6 NASA Lewis IRT Cases

The NASA IRT cases are used to show the impact of the ice roughness, the turbulence model and other parameters on the HTC computation which impact directly the predicted ice shapes. The cases are described in the next section. The impact of several components affecting the icing simulations will be discussed.

4.6.1 Cases properties

In this work, the effects of the integration of the diverse models are studied in comparison with experimental data generated in the NASA IRT [2]. These results allow determining how the code variants can predict specific ice properties, discussed in Section 4.6.2. The differences between the computed results and the experimental ice shapes are assessed, as well as the qualitative distinctions between the experimental ice shapes. The airfoil utilized is a NACA0012. Each test uses the same reference geometry, composed of a constant cross-section in the spanwise direction with no sweep angle. To extract the ice shape data in 2D after an experiment, a small section of the ice growth is cut out and the contour of the ice shape is traced on a cardboard template with a pencil. The pencil tracing is then digitalized. Acquisition errors can appear at this stage and the ice shapes have spanwise variabilities. This is why multiple experimental data at several spanwise sections are collected for a unique test case. A monodispersed droplet size distribution is used. The only qualitative difference observed from LEWICE 2.0 [15] results, when using a 7-bin Langmuir-D distribution, is wider icing limits [2]. The conditions for all the cases used are resumed in Table 4.1.

The series 4XX shows glazed ice cases (except for 425) at different Reynolds numbers, temperatures, icing times and LWC.

Table 4.1 Simulation parameters for the NASA IRT cases [2]

Case	AoA [°]	Chord (m)	Static Pressure (kPa)	U (m/s)	T _∞ (K)	LWC (g/m ³)	MVD (μm)	Icing Time (s)
35	4.0	0.5334	92.06	93.89	260.80	1.05	20.0	372.0
36	4.0	0.5334	92.06	93.89	266.40	1.05	20.0	372.0
401	4.0	0.5334	92.06	102.80	265.37	0.55	20.0	420.0
403	4.0	0.5334	100.00	102.80	262.04	0.55	20.0	420.0
421	4.0	0.5334	100.00	67.10	268.40	1.00	20.0	360.0
425	4.0	0.5334	100.00	67.10	241.51	1.00	20.0	360.0

4.6.2 Metrics for the comparison

Diverse metrics can be employed to compare the ice shapes from numerical simulations to the experiments. For the moment, the comparison is made by a qualitative assessment. More precise metrics can also be used. For this work, the metrics are:

1. The ice limits locations;
2. The orientation of the horns;
3. The maximum ice thickness and its location;
4. The ice thickness at the stagnation point.

The overall ice shape is analyzed as well. The experiments also have their share of variabilities.

4.6.3 Results with standard turbulence models

Ice shapes obtained with the SA one-equation turbulence model and with the $k-\omega$ SST2003 two-equation turbulence model are presented. The main objective is to show baseline results for further improvements as well as the main difference between the two turbulence models with their respective rough wall boundary conditions. Figure 4.5 displays the ice shapes obtained for the NASA IRT cases 35, 36, 401 and 403, which are all glazed ice cases. Small differences in the Reynolds number, the freestream temperature, the liquid water content and the icing time give distinctions for the shapes of the ice accumulated for the cases. Since the roughness of the clean and each layer of ice is unknown, results with three different roughnesses are presented, respectively $k_s/c = [3, 6, 9] \times 10^{-4}$. These three non-dimensionalized roughness heights give the best qualitative results for the ice shapes. As a reference, the equivalent sand grain roughness heights prescribed by Shin *et al.* [90] correlation are respectively $k_s/c = [5.94, 7.52, 7.56, 6.58] \times 10^{-4}$ for cases 35, 36, 401 and 403, which are close to

the employed values. Different numbers of layers are tested. The best compromise between the resolution of the ice shape and the computation time is obtained for six layers.

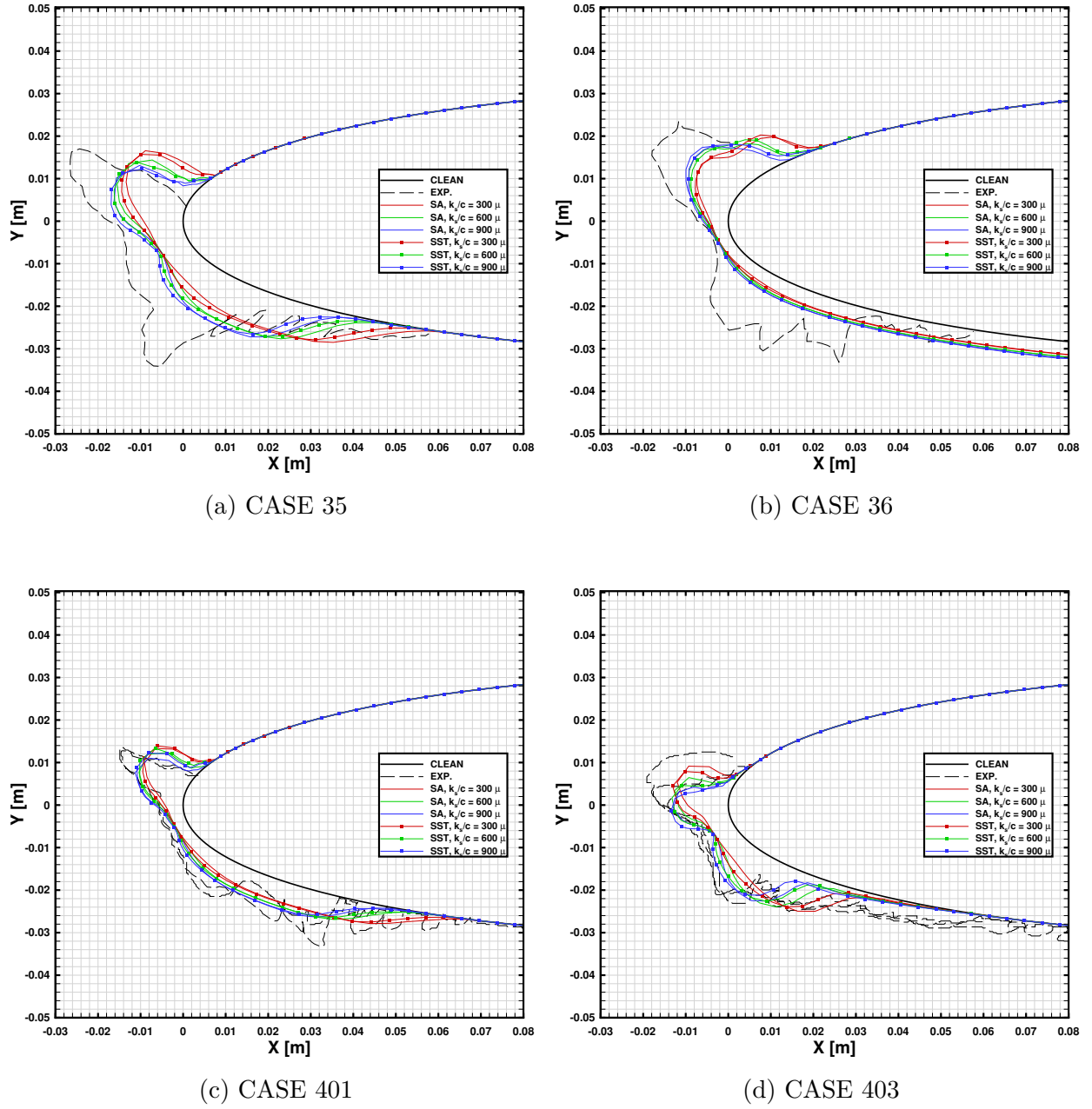


Figure 4.5 Ice shapes obtained for the NASA IRT cases with SA and $k-\omega$ SST2003 (SST) turbulence models for different global roughnesses, compared to experimental results (MVD = $20 \mu\text{m}$, 6 layers)

As these ice shapes serve as a reference for further tests, the issues with the current ice patterns are exposed. For all the cases, both turbulence models give similar results. For case

35, the orientation of the upper horn is well captured, but not the shape of the lower horn. The ice limits are too far toward the trailing edge. The feathers accumulating at the bottom are not seized. For case 36, similar observations are made. The upper ice limit seems to be well obtained but no lower horn is observed. The height of the upper horn is not well seized. For cases 401 and 403, the orientations of the upper horns are well caught and are at their best for the higher roughness. It is hard to conclude on the ice limits on the lower surface and the physical aspect of the ice is not well captured at the bottom, but better results are obtained at lower roughness. The total volume of the ice is in good agreement with the experimental curves for these two cases. It is important to note that extensions for the models will be proposed in the next sections to improve the accuracy of the predicted ice shapes. However, slight changes in the angle of attack or the MVD can also significantly influence the results.

4.6.4 Effect of the number of layers on the ice shapes

Figure 4.6 presents the effect of the number of layers on the ice shapes using an equivalent sand grain roughness $k_s/c = 6 \times 10^{-4}$. Only the results with the SA one-equation turbulence model with the Boeing roughness extension are shown in this section since similar results are obtained with the $k-\omega$ SST2003 model.

It is observed that the ice shapes obtained are not changing significantly when four or six layers are used. Therefore, the hypothesis that six layers can be employed to produce accurate results is confirmed. The fact that the appropriate shapes of the upper horns cannot be obtained can be explained by the number of elements of the surface mesh that is not high enough to precisely define the form of the horns. No air pocket is computed for the ice, partially explaining the differences in the total ice volume compared to the experiments. Also, the experiments are 3D: another choice of the cut section could contain more or less ice. Knowing these deficits, the next results will show the effects of using transitional models, especially on the lower horn, for the ice shapes computations.

4.6.5 Effect of the transitional model on the ice shapes

This section shows the effect of using the SA one-equation and the $k-\omega$ SST2003 two-equation turbulence models coupled with the $\gamma-\tilde{Re}_{\theta t}$ transition extension. The freestream turbulent intensity is fixed at 0.8%, which corresponds to the value observed in the NASA IRT. Figure 4.7 shows the ice shapes for cases 35 and 401, employing transitional models and using the same roughness heights as the ones previously mentioned in Section 4.6.3.

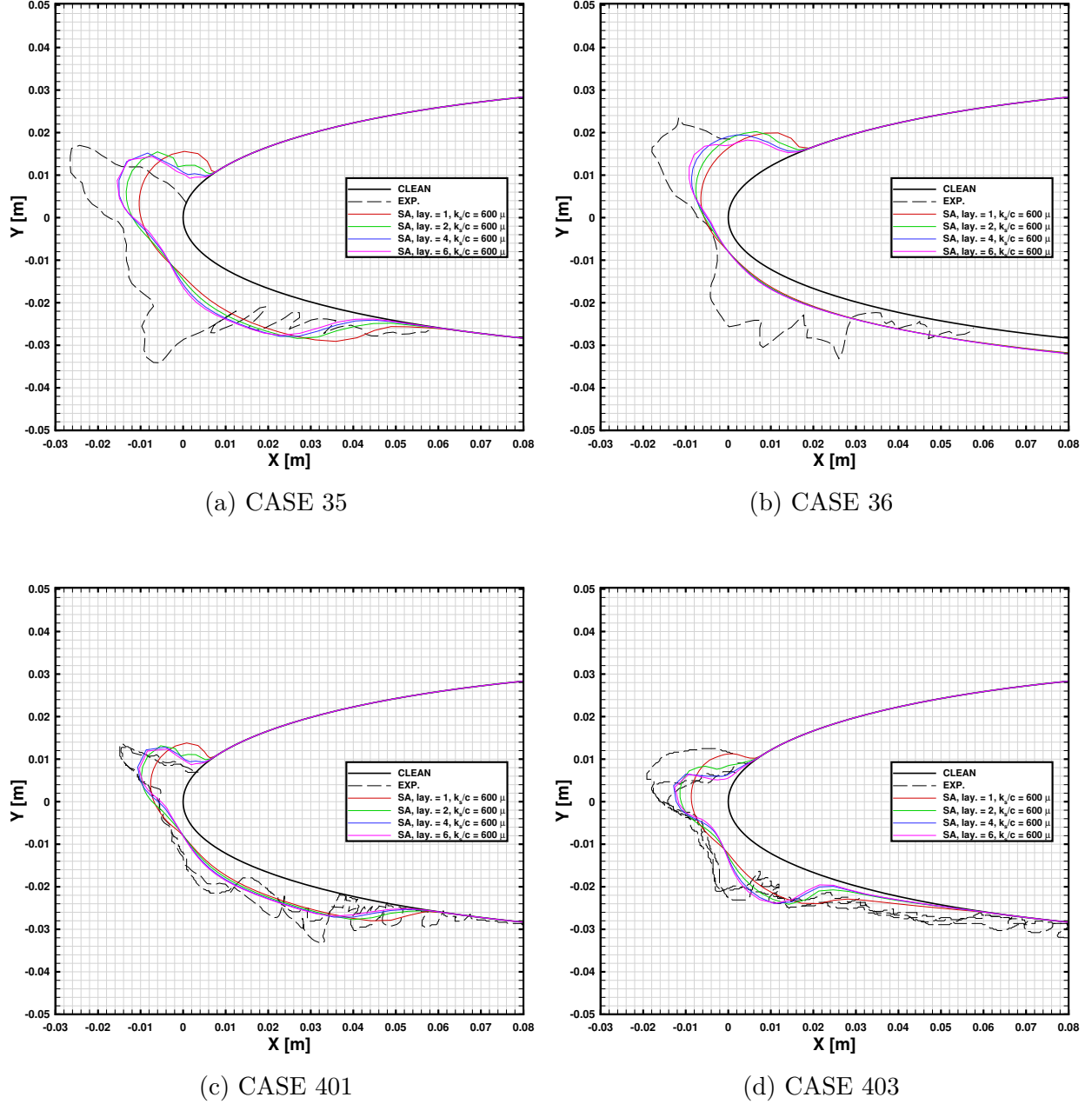


Figure 4.6 Ice shapes obtained for NASA IRT cases with SA turbulence model with different numbers of layers, compared to experimental results ($MVD = 20 \mu m$, $k_s/c = 6 \times 10^{-4}$)

Even if the air velocity has little effect on the ice formation, the Reynolds number determines if a laminar boundary layer is existing or not. It is observed that the ice shapes obtained with a roughness of $k_s/c = 3 \times 10^{-4}$ imply a laminar region that is too wide, giving a displacement of the horns too far toward the trailing edge. The effect of the SA- γ - $\tilde{Re}_{\theta t}$ transitional model is more perceptible for case 35 in Figure 4.7a with $k_s/c = 6 \times 10^{-4}$, where the lower horn is

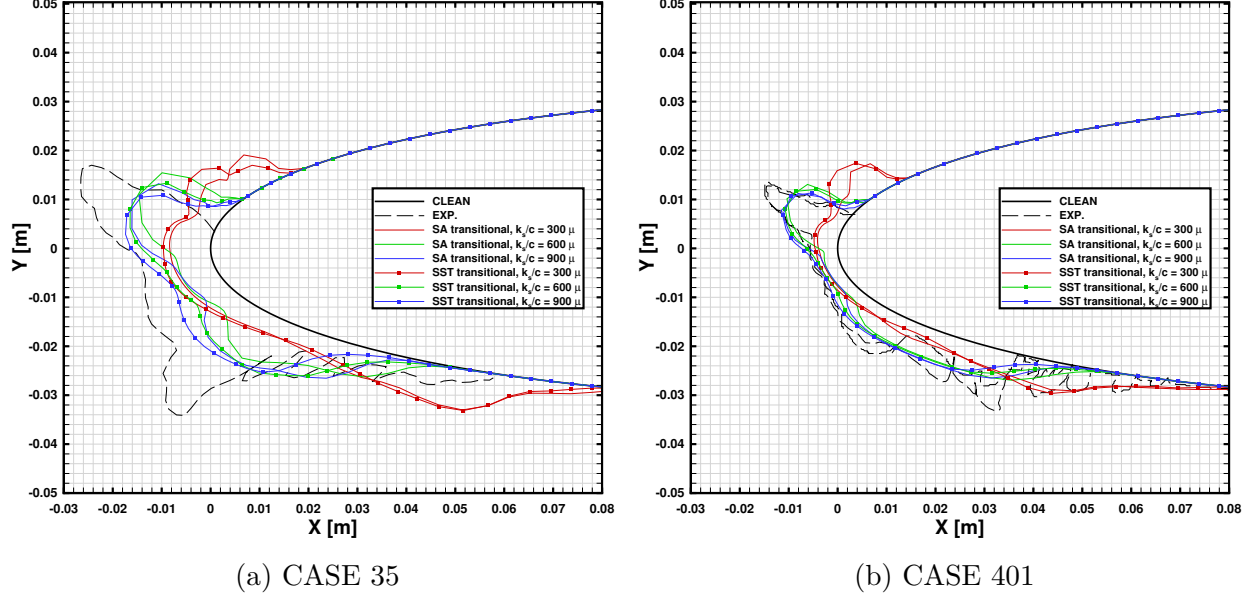


Figure 4.7 Ice shapes obtained for the NASA IRT cases with SA- $\gamma\tilde{Re}_{\theta t}$ (SA transitional) and $k\omega$ SST2003- $\gamma\tilde{Re}_{\theta t}$ (SST transitional) transitional models for different global roughnesses, compared to experimental results ($MVD = 20 \mu m$, 6 layers)

better defined. There is a plateau near the stagnation point that is not captured when using a turbulence model without the transition extension. For case 35, results obtained using $k_s/c = 9 \times 10^{-4}$ with the SA- $\gamma\tilde{Re}_{\theta t}$ transitional model are similar to the results attained with the $k\omega$ SST2003- $\gamma\tilde{Re}_{\theta t}$ transitional model using $k_s/c = 6 \times 10^{-4}$. Therefore, the $k\omega$ SST2003- $\gamma\tilde{Re}_{\theta t}$ transitional model is more sensitive to the given roughness parameter compared to the SA- $\gamma\tilde{Re}_{\theta t}$ transitional model. For case 401 in Figure 4.7b, the impact of the transitional model is less obvious but a flat ice region is still present near the stagnation point and with higher roughness, the bottom horn begins to be captured. Figure 4.8 only shows results employing the SA model to better assess the effect of the transition extension on cases 35 and 421. The roughness values of $k_s/c = 6 \times 10^{-4}$ and $k_s/c = 9 \times 10^{-4}$ are utilized since they give results closer to the experimental data.

It is seen that for $k_s/c = 6 \times 10^{-4}$, Figure 4.8a shows a better definition of the lower horn when using a transition extension. For $k_s/c = 9 \times 10^{-4}$, results with the transitional model are close to the original SA turbulence model. For case 421 in Figure 4.8b, it is observed that the upper horn is thinner and better defined when a transitional model is employed for both roughness values. For case 421, Figure 4.9 shows the HTC along the normalized curvilinear distance from the stagnation point obtained with the SA turbulence model and the SA- $\gamma\tilde{Re}_{\theta t}$ transitional model compared to LEWICE 2.0 [15] numerical results.

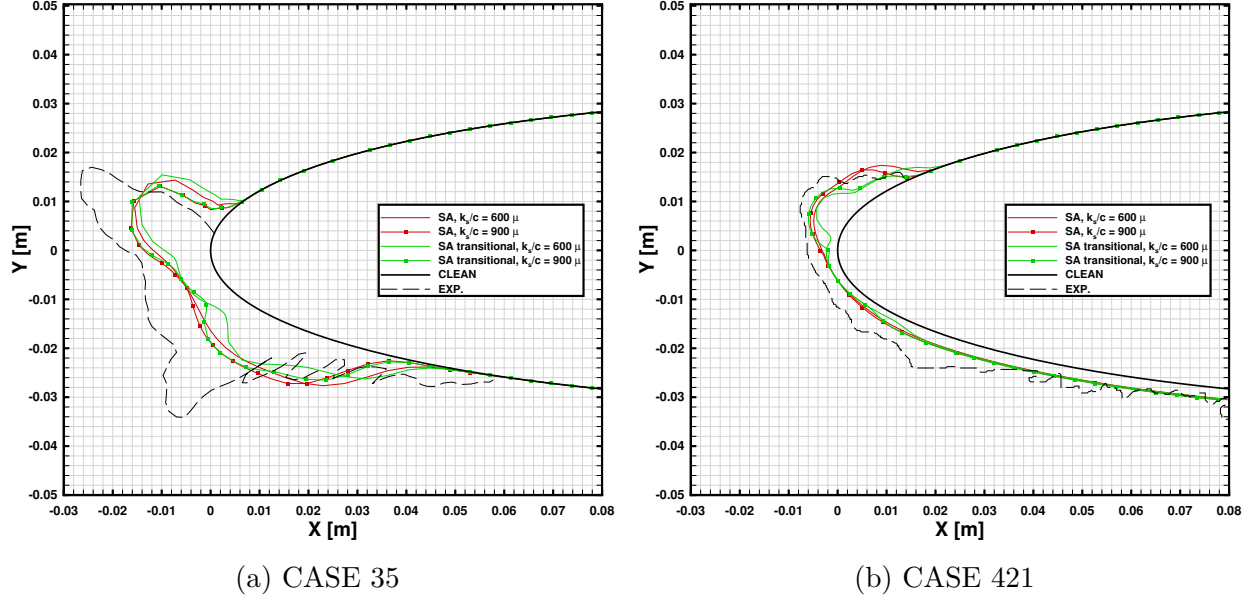


Figure 4.8 Ice shapes obtained for the NASA IRT cases with SA turbulence model and SA- $\gamma\tilde{Re}_{\theta t}$ (SA transitional) transitional model for different global roughnesses, compared to experimental results (MVD = $20 \mu m$, 6 layers)

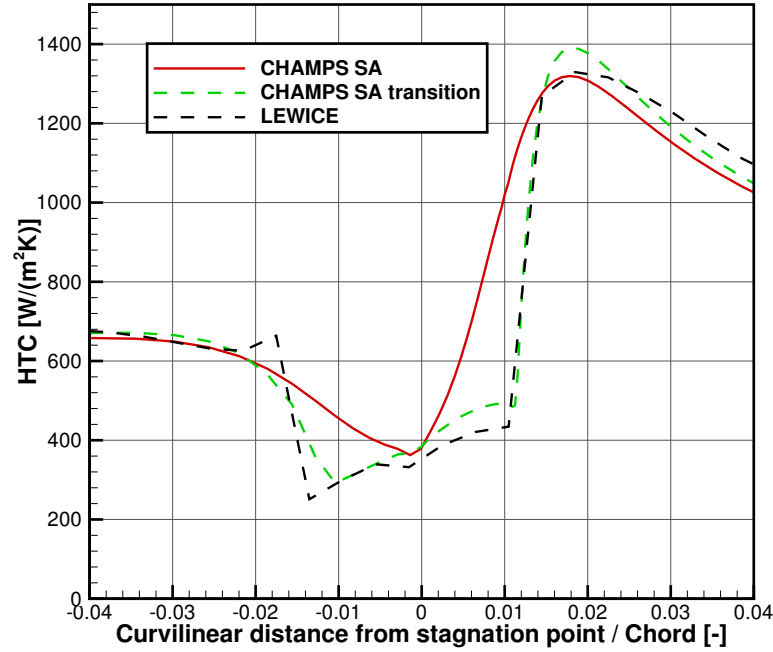


Figure 4.9 Heat transfer coefficient along the normalized distance from the stagnation point with the SA turbulence model and the SA- $\gamma\tilde{Re}_{\theta t}$ (SA transition) transitional model compared to LEWICE numerical results for case 421

Only the region near the stagnation point is analyzed. The angle of attack causes a rapid increase of the convective heat transfer over a short length after the stagnation point. The stagnation point HTC computed by CHAMPS is the same for the SA turbulence model and the SA- γ - $\tilde{Re}_{\theta t}$ transitional model. The results for the SA- γ - $\tilde{Re}_{\theta t}$ transitional model show a laminar HTC region that is of the same length as the numerical results of LEWICE 2.0 [15], which employed a laminar correlation based of Re_{k_s} [91]. The peaks observed are very close between CHAMPS and LEWICE 2.0 [15]. Some differences can be due to the global roughness value utilized, which is $k_s/c = 600 \mu$ for CHAMPS and $k_s/c = 756.5 \mu$ for LEWICE 2.0 [15]. The HTC results for each layer are not analyzed since no numerical or experimental data are available for comparison. The HTC values along the curvilinear distance from the leading edge for each layer will be studied more deeply in Section 5.4 when a local roughness is employed. Appendix B and Appendix C give additional ice shapes and HTC distributions for the NASA IRT cases.

4.6.6 Effect of the freestream turbulence intensity on the ice shapes

In this section, the effect of the freestream turbulent intensity is investigated since its value is rarely measured in wind tunnels. Even if this parameter is measured, transitional models must be calibrated to match experimental data for a given turbulence intensity value. In Figure 4.10, ice shapes of case 35 are presented, when the turbulent intensity varies from 0.2% to 1.2%, which covers a large portion of the turbulent intensities observed in wind tunnels.

For a global roughness of $k_s/c = 3 \times 10^{-4}$, the turbulence intensity value has a great impact on the ice shapes since it modifies the height and the orientation of the horns. When the value of the turbulent intensity is reduced, the horns move downstream. For $k_s/c = 6 \times 10^{-4}$, practically all the results are on top of each other, suggesting a low impact of the turbulence intensity value.

4.7 Problem with the global roughness value imposition

The imposition of a distributed roughness is necessary to have the appropriate scale of the heat transfer and to obtain an ice shape close to the experimental data. When a transitional model is added, the lower horn is captured but could be defined with more accuracy. However, with the global roughness value usually prescribed by conventional global roughness models ($> 600 \mu m$), the flow boundary layer shifts rapidly to a turbulent state and the effect of the transitional model is not observed. More, the global roughness models generally used have

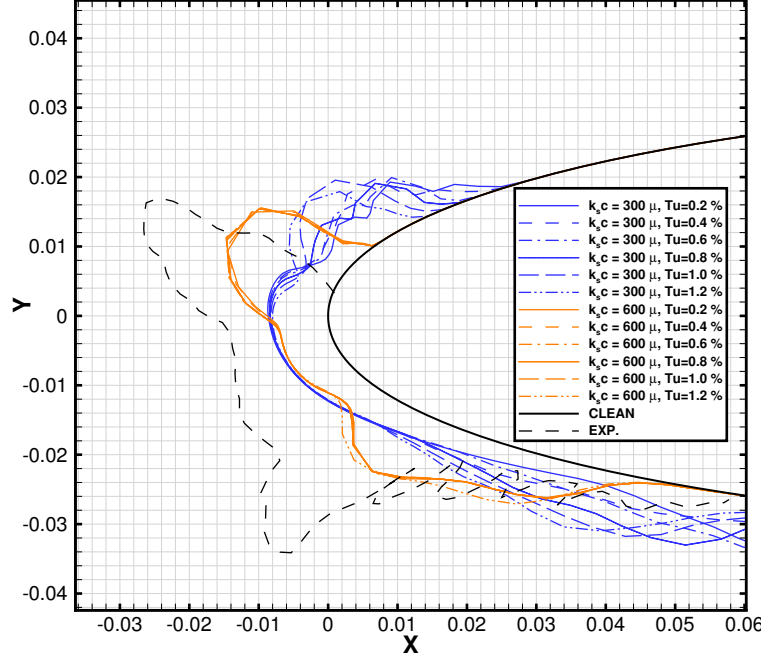


Figure 4.10 Ice shapes obtained for the NASA IRT case 35 with the $SA-\gamma-\tilde{Re}_{\theta t}$ transitional model for different global roughnesses and turbulence intensities, compared to experimental results ($MVD = 20 \mu m$, 6 layers)

been calibrated for first-generation software and not second-generation software. Also, with a global roughness model, it is normally assumed that the surface roughness is the same on the clean geometry and on each layer employed to produce the final ice shape. There is no distinction between the roughness of the water film or the accumulated ice forming the horns.

4.8 Conclusion

This chapter proposes the imposition of roughness extensions to attain physical values for the heat transfer coefficient. Extensions using an equivalent sand grain roughness height for the SA and $k-\omega$ SST models wall boundary conditions are implemented. The extensions are validated and verified with empirical and numerical results for the local skin friction and the heat transfer coefficient. To consider the shift of the transition location due to roughness, a transport equation is added to the transitional models. The employment of such models influences the location of the computed horns for the ice shapes of the NASA IRT airfoil cases. When two horns are present, a laminar region can be computed by the transitional model, capturing the plateau region of the ice and distinguishing the horns.

CHAPTER 5 LOCAL ROUGHNESS CORRELATION FOR TURBULENCE MODELS

In the past years, many specific increments were made to icing codes to improve their accuracy, one of them being increased physics. Some have tried to use a variable ice density to take into account the porosities of the ice [92]. Others have tried to model the stochastic nature of the icing process [24,25]. Recently, variable wall roughness models emerged. These models are either based on the physics of icing or experimental observations and are suitable for glaze conditions with reduced horn growth [93]. Wind tunnel methods have also evolved, so the roughness can be measured on real ice geometries, which can serve to develop new models. This chapter presents the implementation of local roughness models in CHAMPS, their validation and verification and their impact on the prediction of the ice shapes for selected NASA IRT cases.

5.1 Expected effect of the local roughness models

The previous results showed that using a global roughness model triggers a premature transition of the flow very close to the stagnation point, modifying the heat transfer. The effect is to increase the ice accretion near the stagnation point, creating horns that are not oriented like in the experiments for glazed ice cases. For lifting airfoil cases, it is seen that the lower horn is often under-predicted and not in the right position when employing a global roughness. This section relates the transitional models with a local roughness model that promotes a laminar region near the stagnation point, thus decreasing the heat transfer. Moreover, a roughness distribution could also enhance the heat transfer in rough areas with rivulets and beads, combined with the effect of the increase of the heat transfer after the transition onset.

5.2 McClain's models

A first model proposed by McClain *et al.* [94] is based on the airfoil global parameters and stagnation point conditions to provide the maximum roughness value to be used as a global value. This model is not viable when employed for different airplane components. A second model is suggested by McClain *et al.* [6] to compute a local roughness height on an ice-accreted surface. Since a lot of data investigating the effects of cloud scaling parameters, airfoil lifting conditions and freestream static temperatures on the ice accretion roughness were accumulated at the NASA IRT, a predictive empirical roughness model was generated using

these data. Because of the stochastic nature of the roughness of the ice, a physics-directed approach was employed to identify the correlation parameters. The root-mean-square of the roughness scale (mean deviation of the roughness height) is defined as [6]:

$$R_q = \frac{LWC \cdot U \cdot \Delta t_{ice}}{\rho_{ice}} \beta (0.7(1.0 - C_P)) \left(0.34 + \Delta T_{0S}^{2/3} e^{-\Delta T_{0S}/2.25} \right) \quad (5.1)$$

where LWC is the liquid water content, U is the freestream air speed, Δt_{ice} is the accretion time, ρ_{ice} is the ice density, β is the collection efficiency, C_P is the local pressure coefficient and T_{0S} is the stagnation supercooling temperature. McClain *et al.* [6] proposed a new formulation employing the freezing fraction, n , to reduce the computed roughness in the film region:

$$R_q = \frac{LWC \cdot U \cdot \Delta t_{ice}}{\rho_{ice}} \beta (0.7(1.0 - C_P)) n \left(0.34 + \Delta T_{0S}^{2/3} e^{-\Delta T_{0S}/2.25} \right) \quad (5.2)$$

In this work, Eq. (5.1) is referred to as *McClain's model without the freezing fraction* and Eq. (5.2) is referred to as *McClain's model with the freezing fraction*.

The value of the equivalent sand grain roughness, which is the most common roughness scale needed for turbulence models, is not known a priori for a generic roughness distribution. To transform R_q to its equivalent sand grain roughness value, the correlation from Flack and Schultz [95] is used. They analyzed three-dimensional rough surface topographical measurements and linked them to the measured equivalent sand grain roughness describing the surface hydraulically. The correlation is valid for fully rough regimes but has not been validated for transitionally rough regimes. Their analysis indicated that the mean deviation of the roughness height and the skewness of the roughness elevation (s_k) were strongly linked to the equivalent sand grain roughness value. This correlation is:

$$k_s = 4.43 R_q \cdot (1 + s_k)^{1.37} \quad (5.3)$$

The skewness is a way of describing if the roughness has more peaks or valleys. If the peaks are large and isolated, the skewness will be high and positive. On a surface that is pitted, the skewness will be negative. Since this value needs to be measured from the ice shape, McClain *et al.* [6] recommend employing a Gaussian surface distribution, meaning a null value for the skewness.

5.2.1 Verification and validation of the models

To verify and validate the implementation of McClain's models in CHAMPS, a NACA0012 glazed ice case is used. The case was experimentally investigated at the NASA IRT. The chord of the airfoil is 0.5334 m , the AoA is 3° , the freestream speed is 67 m/s , the MVD is $29.5\text{ }\mu\text{m}$, the LWC is 0.6 g/m^3 , the icing time is 94 seconds and the freestream temperature is 268.92 K . The numerical results from McClain *et al.* [6] are based on an inviscid panel method solver to calculate the pressure coefficients. The collection efficiency and freezing fraction are calculated using LEWICE 3.2 [42]. A 7-bin drop-size distribution is employed based on the NASA IRT icing cloud calibration report [96]. For CHAMPS computations, a 7-bin Langmuir-D distribution is used with the proposed MVD. CHAMPS and LEWICE 3.2 (McClain *et al.* [6]) results of R_q along the curvilinear distance from the leading edge are presented in Figure 5.1. The experimental data have been obtained using the Maximum Combined Cross-Section (MCCS) definition by Broeren *et al.* [97] and the self-organizing map approach for the roughness characterization used by McClain *et al.* [98]. Note that the legend carries *without n* and *with n* (n being to the freezing fraction), to respectively refer to the correlation of Eq. (5.1) and Eq. (5.2).

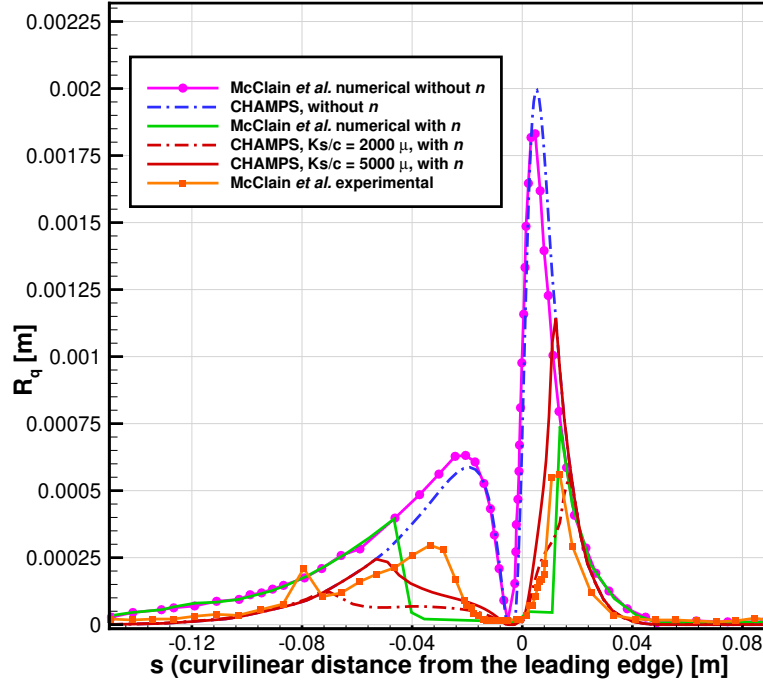


Figure 5.1 Root-mean-square of the roughness scale along the curvilinear distance from the leading edge computed with McClain's roughness models compared with McClain *et al.*'s [6] experimental and numerical results on a NACA0012 glazed ice case (MVD = $29.5\text{ }\mu\text{m}$, $U = 67\text{ m/s}$, $T_\infty = 268.92\text{ K}$)

Numerical results from McClain *et al.* [98] without the freezing fraction track the value of the roughness outside of the limit of the maximum roughness but overestimate the value in the film region appearing for $s \approx [-0.05, 0.02]$. When considering the freezing fraction in the model, no roughness is computed in the film region but the roughness peaks are too far from the leading edge. A film roughness can be present under certain conditions [6]. With both formulations, neither CHAMPS nor LEWICE 3.2 (McClain *et al.* [6]) is able to compute the desired positions of the roughness peaks. When including the freezing fraction in the correlation, CHAMPS underestimates the height of the peaks, while McClain *et al.* [6] overestimate them. This can be due to the definition of the freezing fraction used in both codes or the moment at which it is computed (i.e before or after the application of the roughness formulation in the computation). Two high global sand grain roughness have been employed on the clean airfoil in CHAMPS computations in order to match the freezing fraction values from McClain *et al.* [6]. In this case, only one layer was computed, and the clean airfoil roughness has a significant impact on the freezing fraction distribution along the airfoil. The differences in the results of the two formulations can be explained by the droplet distribution and the mesh, which are not the same between the codes.

The orange curve of Figure 5.1 shows that the experimental roughness varies along the iced surface and has a maximum on each side of the stagnation point. The difference in height between the two local maxima is caused by the angle of attack that was applied to the symmetric airfoil. From other experimental data, local peaks can be observed in the film section, due to the film waves. With McClain’s model of Eq. (5.2), these roughness peaks cannot be present in the film region, since the computed value is directly proportional to the freezing fraction. With Eq. (5.1), the film roughness is largely overestimated.

5.3 Implementation of local roughness models

When including the freezing fraction in the local roughness formulation, several issues affect the icing workflow. The complexity comes from the fact that the local roughness correlation is employed to improve the accuracy of the heat transfer. In a global approach, the roughness is applied to the initial geometry and impacts the boundary conditions of the flow solver. However, the parameters employed in McClain’s formulations are computed in the flow, droplet and thermodynamic solvers. Also, the convective heat transfer is necessary to predict the freezing fraction, which impacts the ice accumulating at a time step, affecting the roughness. The challenge is to assess at which step in the loop the roughness and the freezing fraction need to be computed. To get out of this circular dependency, several approaches are proposed in Figure 5.2.

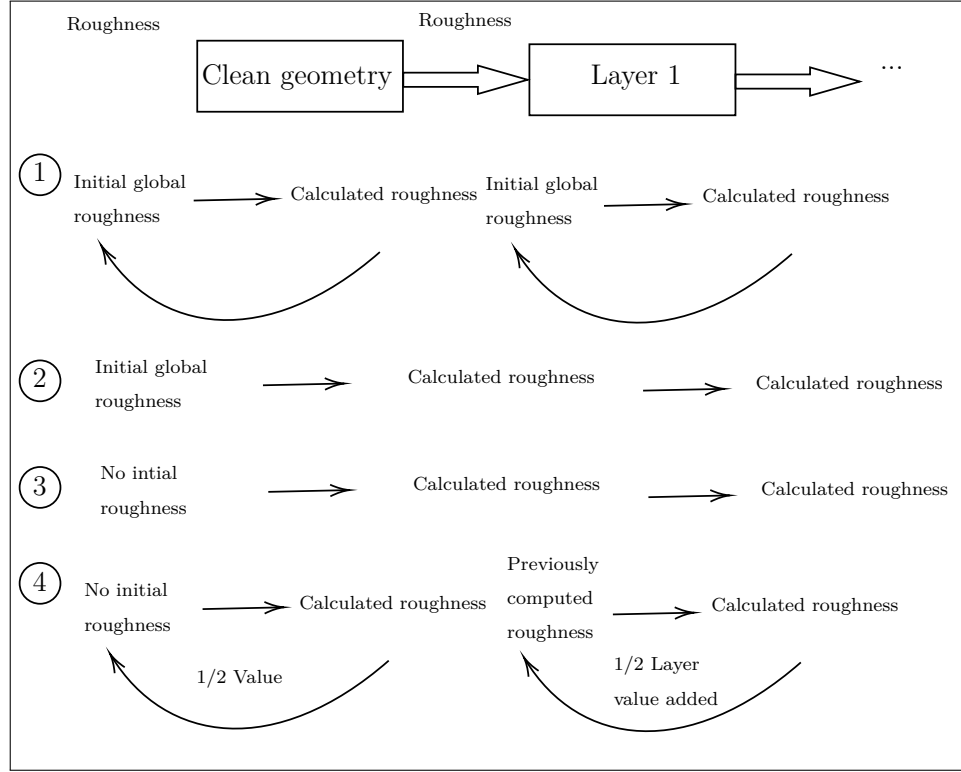


Figure 5.2 Methods to introduce McClain's local roughness models

Approaches 2 and 3 start with either a global roughness on the clean surface or a smooth surface (no roughness). The roughness computed at the end of the initial layer is then projected on the first layer of ice using the mesh connectivity. The shifted cell keeps the same roughness. This is consistent since the roughness is directly proportional to the accretion time, meaning that the roughness projected on the ice corresponds to the roughness at the time of the layer formation. However, since the ice is accumulating in a quasi-steady approach, the ice roughness does not correspond to the mean roughness during the layer accretion step. Normally, on the clean geometry, the global roughness to be imposed is not known: a smooth surface for the initial layer is preferable. However, when the total number of layers is low, using no roughness on the clean geometry underestimates the heat transfer and the initial ice shape. Thus, in this work, a global roughness is used on the clean geometry, corresponding to a value predicted by a global correlation. Referring to Figure 5.2, approach 1 initially computes a layer with a global roughness defined by the user, calculates the local roughness at the end of the layer accretion, then recomputes the layer using the local value of the roughness recently determined. This doubles the computation cost of the process but better defines the first layer, which is important for the rest of the ice accretion process. However, since this reinjects the local roughness values corresponding to the end of the layer

accretion time, it overestimates the roughness. Approach 4 suggests using the accretion time corresponding to half of the layer accretion when computing the roughness. This implies that the mean value of the layer roughness is employed during a layer recalculation.

McClain *et al.* [6] do not use the roughness formulation as an input to their icing code. They employ it to compute the maximum roughness and inject it as a global value until the ice shape transitions from roughness on an airfoil to a full two or three-dimensional ice shape, limiting the global value applied. Thus, the time dependency of the local roughness needs to be limited in order to avoid non-physical values, which has not been done in this work. The model also has never been validated for local employment with turbulence and transitional models.

5.4 Effect of the local roughness models on the ice shapes

This section discusses the impact of using the two McClain's correlations for the local roughness on the ice shapes of the NASA IRT cases 35 and 403. The parameters for these cases are displayed in Table 4.1. Results were generated with four ice layers. For the first layer, a global non-dimensional roughness (k_s/c) of 600μ is employed, as it corresponds to the roughness used in the global roughness ice shapes comparisons. The turbulent intensity of the simulations is 0.8%. Figure 5.3 shows the obtained results when the freezing fraction is not considered in McClain's local roughness correlation as proposed in Eq. (5.1) for cases 35 and 403.

As observed previously in Figure 5.1, the roughness peaks are too close to the stagnation point, and so are the peaks of the convective heat transfer. Therefore, the ice horns are generated too close to the stagnation point. For the lower shape of the ice, in Figure 5.3a, even if ice feathers are not present, the lower section is closer to the experimental data and the lower horn is better defined when a local roughness is employed. For the upper horn, the orientation is better captured without the use of the local roughness correlation. The use of the transitional model for the flow does not seem to impact significantly the global ice shape when this McClain's roughness correlation is employed. In Figure 5.3b, the lower horn seems to be closer to the orientation of the experimental horn when a local roughness is employed, but the same conclusions as for Figure 5.3a can apply to the upper horn. In Figure 5.4, the freezing fraction is included in McClain's local roughness correlation. The same cases are employed to show the effects of the correlation on the ice shapes.

Employing the freezing fraction in the roughness correlation changes the orientation of the horns by moving them farther from the stagnation point. For this roughness formulation, the

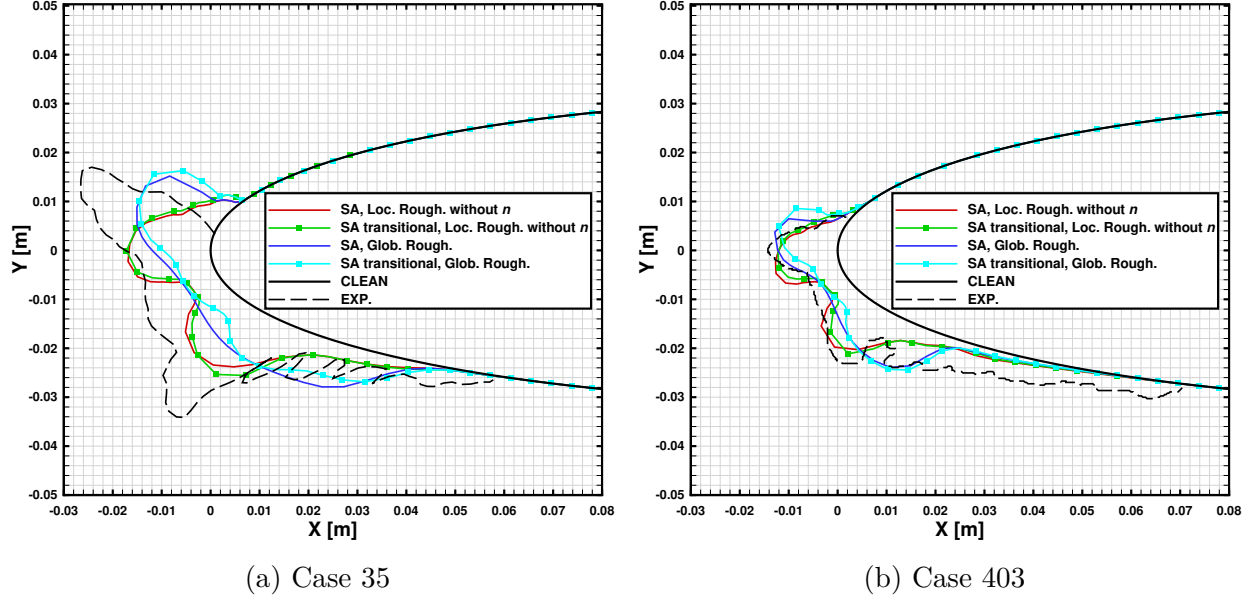


Figure 5.3 Ice shapes obtained for the NASA IRT cases with SA turbulence model and SA- γ - $\tilde{Re}_{\theta t}$ (SA transitional) transitional model and McClain's roughness formulation without the freezing fraction, compared to experimental results (MVD = 20 μm , 4 layers, $k_{s0} = 600 \mu m$)

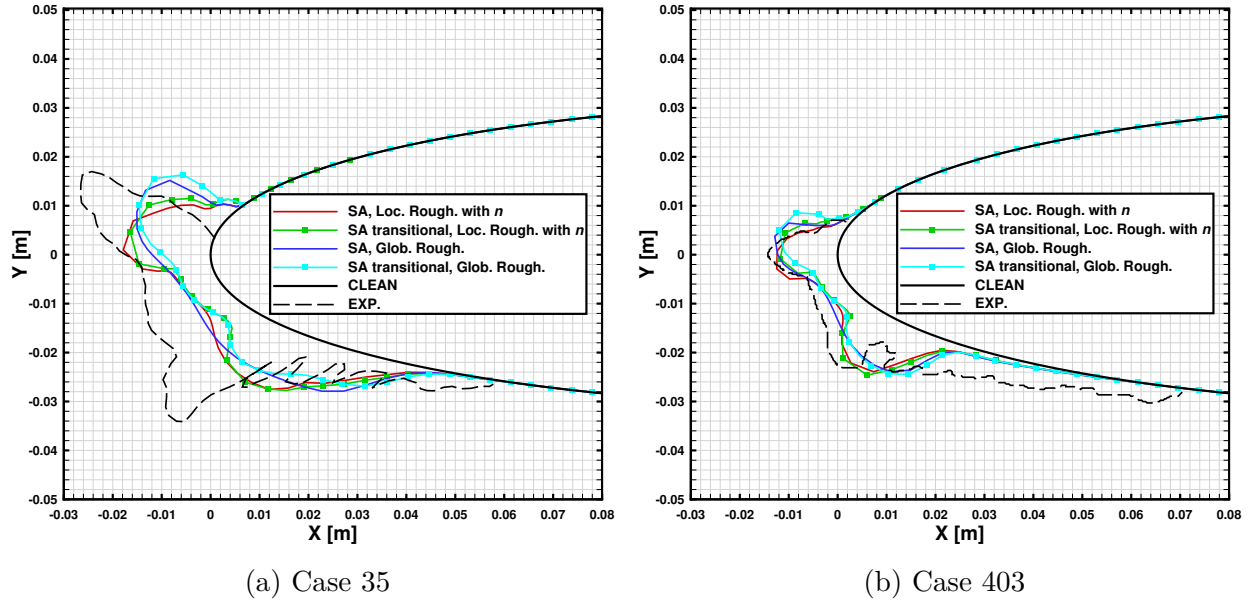


Figure 5.4 Ice shapes obtained for the NASA IRT cases with SA turbulence model and SA- γ - $\tilde{Re}_{\theta t}$ (SA transitional) transitional model and McClain's roughness formulation with the freezing fraction, compared to experimental results (MVD = 20 μm , 4 layers, $k_{s0} = 600 \mu m$)

final ice shape is strongly dependent on the roughness of the clean geometry. The application of the transitional model affects the ice shape contrary to the results in Figure 5.3. It can be argued that in Figure 5.4a, the orientation of the upper horn is better captured when the transitional model is coupled with the local roughness model. For the same case and combination of models, the height of the lower horn is closer to the experimental data and the transitional model makes a difference in the horn orientation. The icing limits are not impacted by the roughness model, nor is the total volume of ice. In Figure 5.4b, the effect of the transitional model near the stagnation point is less visible but still present. For both horns, their orientations seem to be closer to the experiment when using the local roughness model, but still, no ice is captured on the lower section of the airfoil. Based on these observations, the next figures display the height of the ice accreted, the HTC and the local normalized sand grain roughness for each layer of ice against the curvilinear distance from the leading edge for case 35. The ice height corresponds to the ice accumulated for the layer and not the total ice height. Figure 5.5 presents these results when Eq. (5.1) is employed.

For the first layer in Figure 5.5a, as it can be observed by a plateau in the HTC, a laminar region is present on the lower surface. These two peaks of the HTC create two distinctive horns on both sides of the stagnation point. The length of the laminar region is directly due to the global roughness employed on the clean surface. The height of the ice generated follows the HTC aspect until all the film is frozen. In Figure 5.5b, a local roughness is employed to calculate the flow field. The HTC aspect is similar to the previous ice height aspect, while the peaks are increased by the local roughness value. It can be seen that the HTC peaks orient the ice growth direction. The horns on both sides of the stagnation point are of similar aspects and amplitudes.

For layers three and four, the peaks of the HTC are still higher on the upper surface, and the growth of the horns is of the same amplitude for both. As expected, the roughness on the lower region is of inferior amplitude than the upper region. Between each cell, the roughness local value changes greatly, meaning a loss in the precision of the captured peak values. This can be improved by adding more cells based on the surface curvature. The value of the peak of the roughness, normalized by the airfoil chord is close to 0.08 on the last layer. Limits are present for the values that can be considered by turbulence and transitional models. Also, there is an ambiguity when calculating a surface roughness on what is considered a microscopic surface roughness and what is considered to be the curvature of the surface. For example, ONERA [50] uses a global roughness of 0.1 percent of the chord for their computations, which is close to a hundred times less than the peak of the computed local roughness in this case. This overprediction of the roughness can result in an overprediction of the HTC, which can move the horns toward the stagnation point. Therefore, even if the

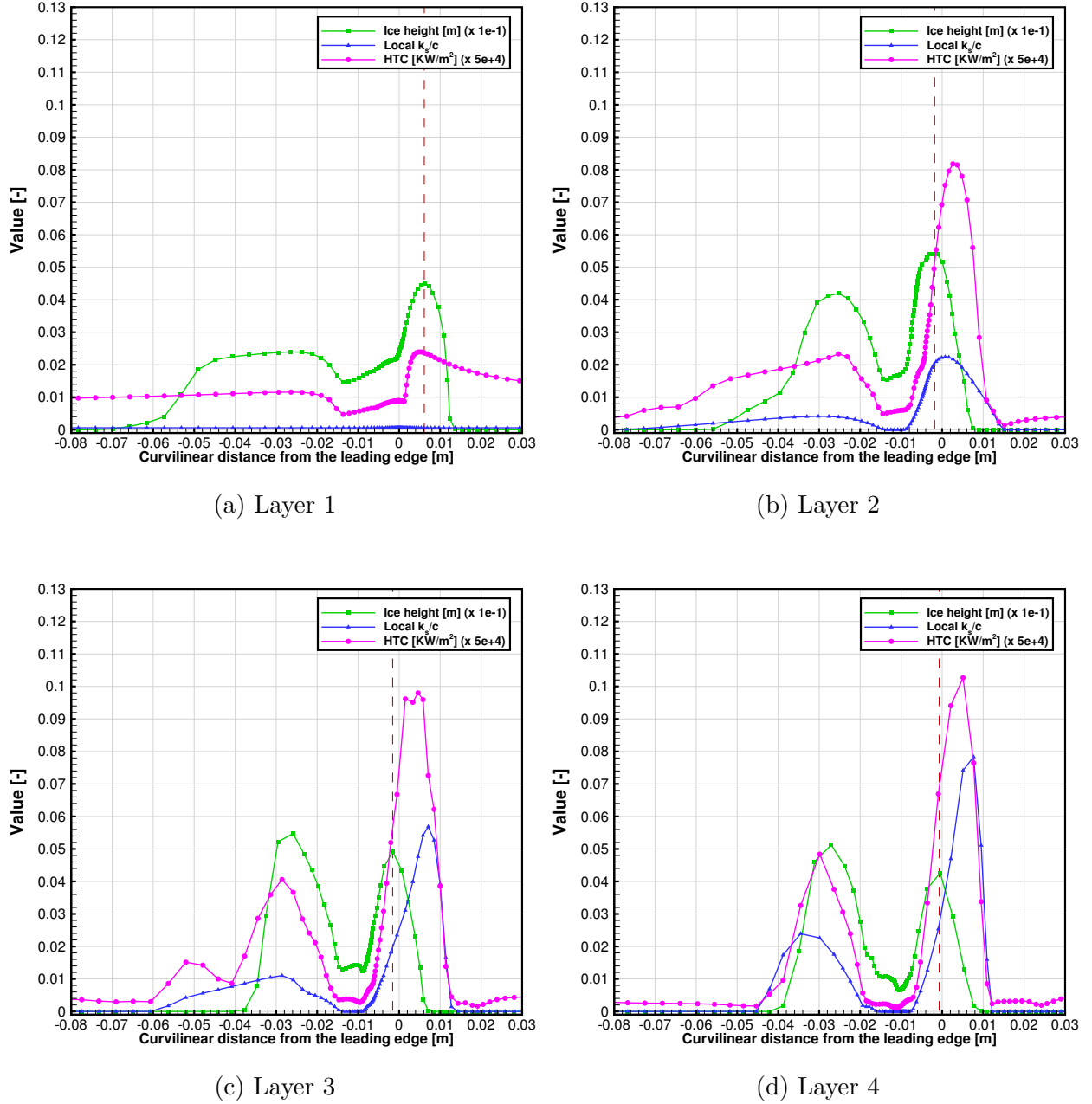


Figure 5.5 Evolution per accretion layer of ice thickness, HTC and local roughness for case 35 with the $SA-\gamma-\tilde{Re}_{\theta t}$ transitional model, McClain's local roughness model without the freezing fraction ($k_{s0} = 600 \mu m$)

aspect of the roughness is adequate, its amplitude can affect the orientation of the horns in an undesirable way. Moreover, the transition lengths computed can impact the HTC peaks, giving different ice shapes. Min and Yee [99] suggest that the HTC on the lower side of an airfoil with a positive AoA, having smaller pressure gradients than the upper surface, is more

impacted by the local roughness model and the transitional model. The lack of experimental measurements of the effects of the ice roughness on heat transfer limits the validation of the heat transfer modeling. Figure 5.6 presents similar results when including the freezing fraction in the local roughness computation, like in Eq. (5.2).

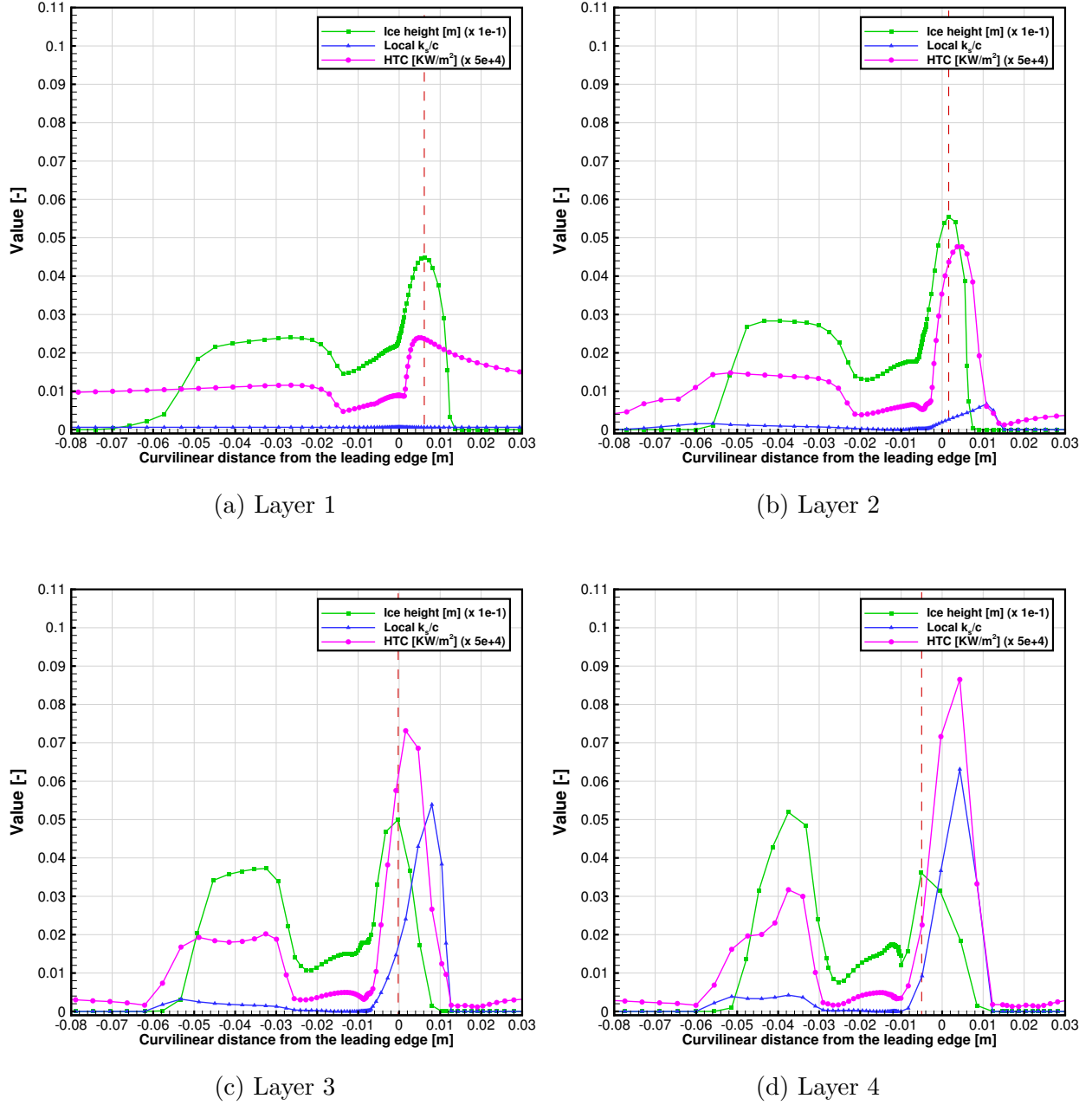


Figure 5.6 Evolution per accretion layer of ice thickness, HTC and local roughness for case 35 with the SA- γ - $\tilde{Re}_{\theta t}$ transitional model, McClain's local roughness model with the freezing fraction ($k_{s0} = 600 \mu m$)

Compared to Figure 5.5, Figure 5.6 generally shows a larger laminar region for each layer. The position and the maximum amplitude of the local roughness on the upper surface are close to the values computed for each layer of Figure 5.5. The maximum roughness on the lower surface is close to four times less than the value of Figure 5.5 for each layer and its position is far more downstream. This influences the HTC, and thus the lower horn is more spread on the lower surface. The plateau region between the two ice horns is close to 2 *mm* using the local roughness model of Eq. (5.2), when it is close to 1 *mm* in Figure 5.5, using Eq. (5.1). The heights of the two ice horns are similar to the ones obtained in Figure 5.5d for layer four.

5.5 Conclusion

Based on the results obtained in this chapter, including the freezing fraction in McClain's local roughness correlation shows promising results to obtain the appropriate orientations for the two horns in glazed ice cases. The models have been verified and validated with a conventional NACA0012 airfoil case. However, using a local roughness slightly shifts the upper horn orientation toward the stagnation point when its orientation is generally well predicted using only a global roughness model. For the lower horn, the local roughness model helps to define its height and orientation. McClain's model presented in Eq. (5.2) has the advantage of calculating no roughness near the stagnation point, which creates a laminar region when a transitional model is used. Doing so, the plateau between the two horns is better characterized. Some calibrations still need to be made with McClain's models to define the roughness for the film region, improving the stagnation thickness and predicting the adequate positions of the roughness peaks. To do so, larger databases should be used to calibrate the models and the film properties could be considered as proposed by Fortin *et al.* [51].

CHAPTER 6 CONCLUSION

This chapter concludes with the observations made during this work. Summaries concerning the use of the transitional models, the global roughness models and the local roughness models are carried out. Then follows a concise assessment of the limitations of the research and recommendations for future improvements of the work.

6.1 Summary of works

While the rime ice accretion predictions for second-generation icing codes follow their experimental equivalents, these icing solvers still have difficulties predicting glazed ice shapes, particularly in the presence of ice horns. CHAMPS, the RANS multi-physics solver developed at Polytechnique Montreal, behaves similarly. While many improvements can be made to second-generation codes, this work focused on the upgrade of the flow solver for icing simulations by increasing the accuracy of the predicted heat transfer coefficient. To compute a physical value for the heat transfer, the boundary layer must be defined in its correct state (laminar or turbulent). This characterizes the freezing rate of the water running back or impacting the surface. The boundary layer is defined by the flow conditions, but also by the geometry shape and its surface aspect, like its roughness. The transition of the boundary layer was tackled by the implementation of transitional RANS models in CHAMPS. Since a global roughness is generally implemented in the literature, which rapidly triggers the transition of the boundary layer, local roughness models were proposed. The new models reduce the roughness in the film region, allowing to capture the laminar boundary layer of the flow near the stagnation point of an iced airfoil, thereby increasing the accuracy of the computed heat transfer.

6.1.1 Implementation of transitional RANS models

The fully turbulent Spalart-Allmaras one-equation turbulence model [37] was initially implemented in CHAMPS. For icing simulations, this model was employed to compute the flow field around the given geometry. Work has been done to introduce the k - ω SST two-equation turbulence model [60] and its variants in CHAMPS. It permits doing ice-shape comparisons with other codes using the same turbulence model for the flow computation. Since the boundary layer state greatly affects the computed friction and heat transfer coefficients, workflow accuracy can be improved by implementing transitional RANS models. The effect

is to reduce the skin friction and heat transfer coefficients for laminar regions. To do so, the $\gamma\text{-}\tilde{Re}_{\theta t}$ extension [72] was added to the $k\text{-}\omega$ SST2003 model. It was then slightly modified to be added to the SA model. This triggers the RANS model only in turbulent regions. The turbulence models were verified against CFL3D [64] and FUN3D [65] numerical results on a Flat Plate case. Since no standard verification cases existed for transitional models, validation has been made against experimental data obtained for an NLF0416 test case from the literature [73], showing transition points close to experimental observations for both models.

6.1.2 Implementation of global roughness models

The previous CHAMPS icing solver could only use the one-equation Spalart-Allmaras model with the Boeing roughness extension [78] for the wall boundary condition. This extension takes the equivalent sand grain roughness as the roughness scale parameter. The Aupoix [82] roughness extension, based on Colebrook and White [83] results, was added to the $k\text{-}\omega$ SST2003 roughness model to consider the increase of the friction coefficient and better predict the heat transfer. The friction coefficient shift was validated against the empirical correlation by Mills and Hang [76] on a Flat Plate for roughnesses in the fully rough and transitionally rough regimes. For the transitional RANS models, this modification is not enough to predict the effect of the roughness on the flow. In transitionally rough and fully rough regimes, the roughness has the effect of triggering the transition to a turbulent regime closer to the stagnation point. To do so, an additional transport equation proposed by Langel *et al.* [88] was added to the transitional model to transport the effect of the roughness in the field. The model was calibrated for the $k\text{-}\omega$ SST2003- $\gamma\text{-}\tilde{Re}_{\theta t}$ model but was also added to the SA- $\gamma\text{-}\tilde{Re}_{\theta t}$ model. Since the results are generated with the SA- $\gamma\text{-}\tilde{Re}_{\theta t}$ model, verification and validation have been made for this model against numerical results of Langel *et al.* [88] and experimental results of Feindt [89] for the zero pressure gradient Flat Plate with varying sand grain roughnesses. The NASA IRT cases [2] were utilized to show the impact of the roughness, the choice of the turbulence model and other parameters on the ice shapes. Both SA and $k\text{-}\omega$ SST2003 models gave similar results for the same roughness input. When a typical value of roughness was applied, laminar regions appeared in some cases, affecting the heat transfer and the generation of ice horns.

6.1.3 Implementation of local roughness models

While analyzing experimental heat transfer results on clean surfaces in icing flow conditions, a plateau can appear near the stagnation point, suggesting a laminar boundary layer in this area, limiting the heat transfer. When coupling transitional RANS models to a global

roughness value, the transition was rapidly triggered and practically no laminar region was computed in most of the cases. Also, nearly no experimental assessment of the heat transfer coefficient has been done for subsequent layers of ice. Glazed ice physics suggests that the film region has a very low roughness value near the stagnation point. Farther from the stagnation point, beads and rivulets appear, creating abrupt increases and decreases in the roughness height. To capture these effects, McClain’s local roughness models have been implemented in CHAMPS [6]. These models are based on the local flow, droplet and thermodynamic properties at the wing surface, using or not the local freezing fraction and define the roughness in the film region. These models were verified and validated against numerical and experimental results from McClain *et al.* [6]. The effect of the implementation of such models, coupled with turbulence and transitional RANS model was assessed by using the NASA IRT cases. The results indicated that i) the value of the local roughness strongly impacts the surface heat transfer and the orientation of the ice horns, and ii) the laminar region appearing on an ice shape can be broadened by the use of a local roughness, giving a better distinction between the horns.

6.2 Limitations

Many technical improvements were added to CHAMPS. However, some limitations still remain with the new features. First, to use a global roughness value, the mesh must be refined to have an appropriate y^+ at the wall. The recommended value in the literature is around 0.1, but a value under 1 gives similar results. Also, to improve the quality and the definition of the horns computed for an icing case, a high number of cells must be used for the surface mesh. If a low number of cells is used for the local roughness, this creates jumps in the surface solution. If this is the case, cells should be added to the surface mesh based on the curvature of the ice geometry. This is not yet available in CHAMPS. For the use of the turbulence model, only the SA model was kept for the icing cases using a local roughness model (with and without the transitional equations). This choice has been made for accuracy, a lower calculation time and a better residual convergence compared to the $k-\omega$ SST2003 turbulence model and its transitional extension. For the icing cases, six layers have been employed for the computations in Chapter 4, which is a good compromise between the computation time and the accuracy for the selected mesh. When using a local roughness, results have been generated with four icing layers due to convergence problems.

Moreover, some parameters were left to the discretion of the user when doing the icing simulations. One of these parameters is the ambient turbulent intensity employed by the SA- γ - $\tilde{Re}_{\theta t}$ transitional model for the icing simulation. The turbulent intensity was chosen to

be close to the one in the NASA IRT. It has been shown that for moderate to high values of surface roughness, the turbulence intensity has close to no influence on the final ice shape. However, at lower surface roughness, it has a great influence on the laminar boundary layer forming on the ice shape. Thus, the effect of the turbulent intensity could have been studied with the local surface roughness. The effect of the clean surface roughness could have been studied in more depth when a local surface roughness was used, as the first layer of ice has an important influence on the final ice shape. Since a lower number of layers was employed, an initial global roughness was used, corresponding to the optimal value tested when only a global roughness value was employed for each icing layer.

Furthermore, more icing cases could have been utilized to show the impact of the local roughness model. In selected icing cases, the total experimental accumulated ice often seems of a larger volume than the predicted accumulated ice. This suggests that additional physics should be added to the models.

An important limitation of the work is that all the selected test cases were 2D. Other icing phenomena are involved in 3D cases. Fortin *et al.* [51] proposed different ice geometrical aspects in 3D like the formation of beads, rivulets and film waves. The current flow, droplet, thermodynamic and roughness models use local parameters and are extensible to 3D. However, for the roughness, the models have not been validated nor calibrated for 3D icing.

6.3 Future research

As the limitations of the current icing software have been discussed in the previous section, this one suggests solutions to improve CHAMPS regarding these limitations.

6.3.1 Droplet solver and Supercooled Large Droplets (SLD)

The current version of CHAMPS used in this work accounts for the droplet size distribution and the droplet deformation through the source terms. However, splashing, droplet breakup, droplet re-injection and coagulation are not considered. These phenomena influence the solution for large droplets, i.e SLD [100].

6.3.2 Thermodynamic model

CHAMPS currently uses the Modified Iterative Messinger model [19], which is fast and robust. The implementation of an improved thermodynamic model inspired by the work of Myers *et al.* [28] is suggested. This one accounts for the pressure gradients, gravity,

and surface tension in the water film, and uses a variable freezing fraction throughout the layer accretion process. This can impact the computed heat transfer and a variable freezing fraction can be employed while computing the local roughness in the thermodynamic solver. An internal loop can therefore be added for the local roughness computation, based on the change of the freezing fraction.

6.3.3 Stochastic approach for icing

Recent developments in CHAMPS are made to solve the stochastic ice accretion on an advancing front grid [25]. The impingement and freezing processes are performed with probabilities obtained from the droplet trajectory and thermodynamic modules, respectively, which are compared against pseudo-random numbers generated with a uniform distribution. The ice density is shown to change along the surface, which is expected in real ice experiments. Additional physics is captured, like ice feathers generation. Including more accurate transitional models and local roughness models could add even more physics to this approach.

6.3.4 Thermodynamic solver and geometry evolution recalculation

The flow calculation and the droplet collection efficiency calculation are the most expensive aspects of each ice layer step. However, the thermodynamic module and the geometry evolution are considered low-cost steps. A technique that could perhaps be employed is to use a unique flow and droplet field solution and a smaller icing time step for the thermodynamic and geometry evolution solvers [101]. These latter are called several times per icing layer and the collection efficiency is recomputed with the updated surface normal vectors. In doing so, solutions similar to five or ten layers solutions could be achieved with a unique layer simulation, reducing the computational costs and removing the residual convergence problem for the flow computed with the local roughness.

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APPENDIX A TURBULENCE AND TRANSITIONAL MODELS

Developments for the SA model

The extended developments are listed below:

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = P_{\tilde{\nu}} - D_{\tilde{\nu}} + \frac{1}{\sigma} \left[\frac{\partial}{\partial x_j} \left[(\nu + \tilde{\nu}) \frac{\partial \tilde{\nu}}{\partial x_j} \right] + c_{b2} \frac{\partial \tilde{\nu}}{\partial x_i} \frac{\partial \tilde{\nu}}{\partial x_i} \right] \quad (\text{A.1})$$

$$P_{\tilde{\nu}} = c_{b1}(1 - f_{t2})\tilde{S}\tilde{\nu} \quad (\text{A.2})$$

$$D_{\tilde{\nu}} = \left[c_{w1}f_w - \frac{c_{b1}}{\kappa^2}f_{t2} \right] \left(\frac{\tilde{\nu}}{d} \right)^2 \quad (\text{A.3})$$

The eddy viscosity is then computed with the following:

$$\nu_t = \tilde{\nu}f_{\nu1} \quad (\text{A.4})$$

$$f_{\nu1} = \frac{\chi^3}{\chi^3 + C_{\nu1}^3} \quad (\text{A.5})$$

$$\chi = \frac{\tilde{\nu}}{\nu_t} \quad (\text{A.6})$$

Note that c_{b1} , c_{w1} , c_{b2} and κ are constant and $f_{\nu1}$, f_w and f_{t2} are functions.

The boundary conditions are the following:

$$\tilde{\nu}_{wall} = 0, \quad \tilde{\nu}_{farfield} = 3\tilde{\nu}_{\infty} : to : 5\tilde{\nu}_{\infty} \quad (\text{A.7})$$

Developments for the $k - \omega$ SST model

The model uses a blending function to switch from the $k\epsilon$ model in the freestream to the $k\omega$ model when approaching a wall. The model is composed of two transport equations to solve the eddy viscosity comparatively to one of the SA model. The first one is for the kinetic energy (k) and the second is for the specific turbulence dissipation rate (ω):

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_j k)}{\partial x_j} = P - \beta^* \rho \omega k + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right] \quad (\text{A.8})$$

$$\frac{\partial(\rho \omega)}{\partial t} + \frac{\partial(\rho u_j \omega)}{\partial x_j} = \frac{\gamma}{\nu_t} P - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[(\mu + \sigma_{\omega} \mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho \sigma_{\omega 2}}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j} \quad (\text{A.9})$$

The eddy viscosity is then computed with the following:

$$\nu_t = \frac{k}{\omega} \quad (\text{A.10})$$

The boundary conditions, when coupled with γ - $\tilde{Re}_{\theta t}$ equations, are as follows:

$$k_{wall} = 0, \quad \omega_{wall} = 60 \frac{\nu}{\beta_1 d^2} \quad (\text{A.11})$$

$$k_{farfield} = \frac{3}{2} (TuU)^2, \quad \omega_{farfield} = \frac{\rho k}{\mu_t} \quad (\text{A.12})$$

With β_1 a model constant.

Developments for the transitional extension for turbulence models

The γ - $\tilde{Re}_{\theta t}$ transition was originally coupled with the $k\omega$ - SST -2003 turbulence model. Later it was coupled with the SA . The model uses the intermittency (γ) to control the production of turbulence in the boundary layer and the transition momentum thickness Reynold number ($\tilde{Re}_{\theta t}$) to trigger the intermittency. The local flow is fully turbulent when $\gamma = 1$ and fully laminar when $\gamma = 0$. The two equations are the following:

$$\frac{\partial(\rho\gamma)}{\partial t} + \frac{\partial(\rho u_j \gamma)}{\partial x_j} = P_\gamma - E_\gamma + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_f} \right) \frac{\partial \gamma}{\partial x_j} \right] \quad (\text{A.13})$$

$$\frac{\partial(\rho \tilde{Re}_{\theta t})}{\partial t} + \frac{\partial(\rho u_j \tilde{Re}_{\theta t})}{\partial x_j} = P_{\theta t} + \frac{\partial}{\partial x_j} \left[\sigma_{\theta t} (\mu + \mu_t) \frac{\partial \tilde{Re}_{\theta t}}{\partial x_j} \right] \quad (\text{A.14})$$

$$P_\gamma = F_{length} c_{a1} S \sqrt{\gamma F_{onset}} \rho (1 - c_{e1} \gamma) \quad (\text{A.15})$$

$$E_\gamma = c_a 2 \Omega F_{turb} \rho \gamma (c_{e2} \gamma - 1) \quad (\text{A.16})$$

$$P_{\theta t} = \rho \frac{c_{\theta t}}{t} (1 - F_{\theta t}) (Re_{\theta t} - \tilde{Re}_{\theta t}) \quad (\text{A.17})$$

$$F_{onset1} = \frac{Re_\nu}{2.193 Re_{\theta c}} \quad (\text{A.18})$$

$$F_{onset2} = \min(\max(F_{onset1}, F_{onset1}^4), c_{opt4}) \quad (\text{A.19})$$

$$F_{onset3} = \max(c_{opt1} - \frac{1}{2.5^3} RT^3, 0) \quad (\text{A.20})$$

$$F_{onset} = \max(F_{onset2} - F_{onset3}, 0) \quad (\text{A.21})$$

The boundary conditions are the following:

$$\frac{\partial \gamma}{\partial n}|_{wall} = 0, \quad \gamma_{farfield} = 1 \quad (\text{A.22})$$

$$\frac{\partial \tilde{Re}_\theta}{\partial n}|_{wall} = 0, \quad \tilde{Re}_{\theta t, farfield} = \begin{cases} (1173.51 - 589.428Tu_\infty + 0.2196Tu_\infty^{-2}) & \text{if } Tu_\infty \leq 1.3, \\ 331.50(Tu_\infty - 0.5658)^{-0.671} & \text{if } Tu_\infty > 1.3 \end{cases} \quad (\text{A.23})$$

The turbulence intensity is computed with the following equation for the $k\omega$ - γ - $\tilde{Re}_{\theta t}$ model:

$$Tu = 100 \frac{\sqrt{2k/3}}{U} \quad (\text{A.24})$$

Transition criterion

For the $k\omega$ - γ - $\tilde{Re}_{\theta t}$ model, the controlled decay correction is used in all cases and the values of the freestream conditions for $\beta = \mu_t/\mu_l$ are specified. All simulations for the SA - γ - $\tilde{Re}_{\theta t}$ model use $\tilde{\nu}/\nu = 3$, as recommended by Spalart and Allmaras. Transition locations along the x axis are computed using the following criterion for both models:

$$x_{tr}(x) = \max \left(\frac{dC_f(x)}{dx} \right) \quad (\text{A.25})$$

APPENDIX B ADDITIONAL ICE SHAPES RESULTS

This appendix shows additional ice-shape results, for IRT cases that have not been covered in this work.

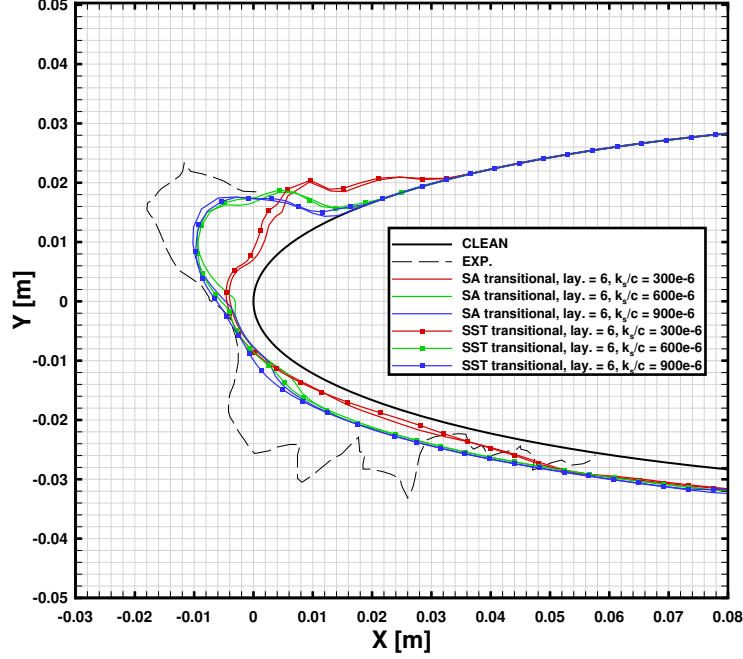


Figure B.1 Ice shapes obtained for NASA IRT case 36 with SA- γ - $\tilde{Re}_{\theta t}$ (SA transitional) and k - ω SST2003- γ - $\tilde{Re}_{\theta t}$ (SST transitional) transitional models for different global roughness, compared to experimental results (MVD = 20 μm , 6 layers)

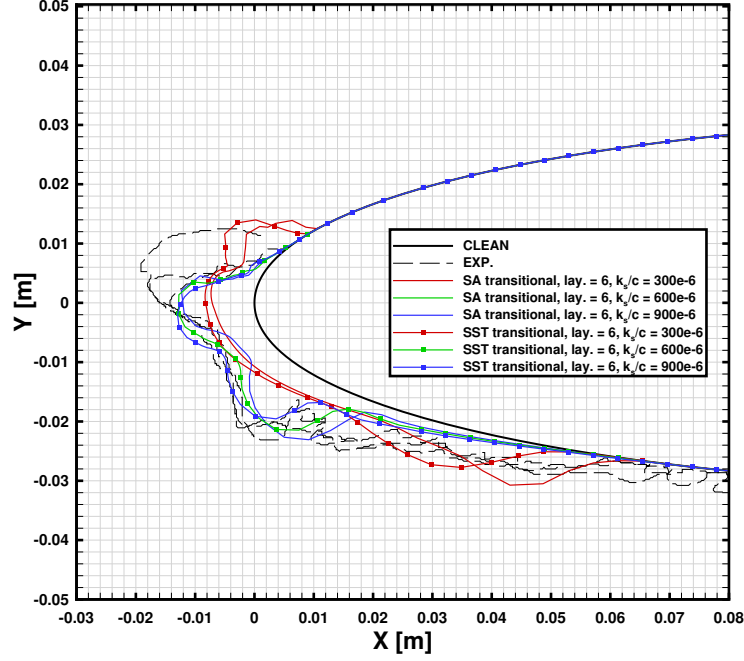


Figure B.2 Ice shapes obtained for NASA IRT case 403 with SA- γ - $\tilde{Re}_{\theta t}$ (SA transitional) and k - ω SST2003- γ - $\tilde{Re}_{\theta t}$ (SST transitional) transitional models for different global roughness, compared to experimental results (MVD = $20 \mu m$, 6 layers)

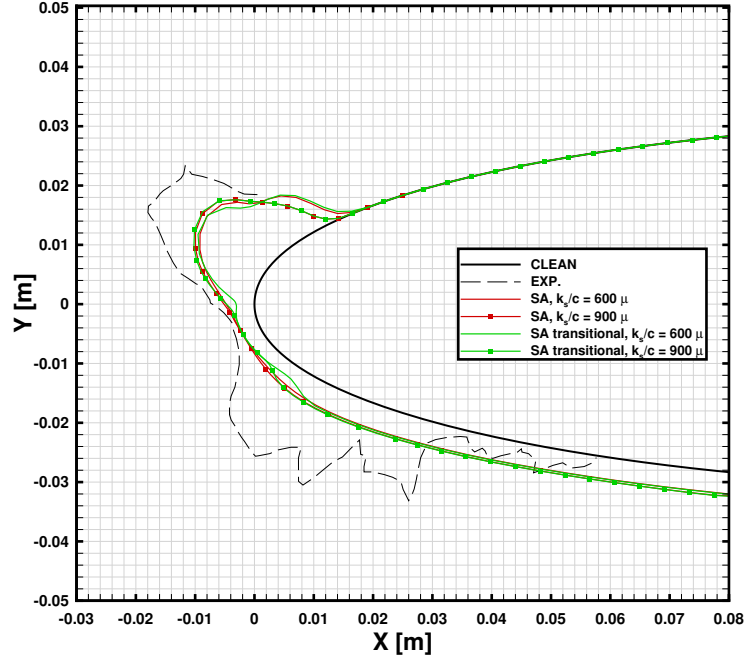


Figure B.3 Ice shapes obtained for NASA IRT case 36 with SA turbulence model and SA- γ - $\tilde{Re}_{\theta t}$ (SA transitional) transitional model for different global roughness, compared to experimental results (MVD = $20 \mu m$, 6 layers)

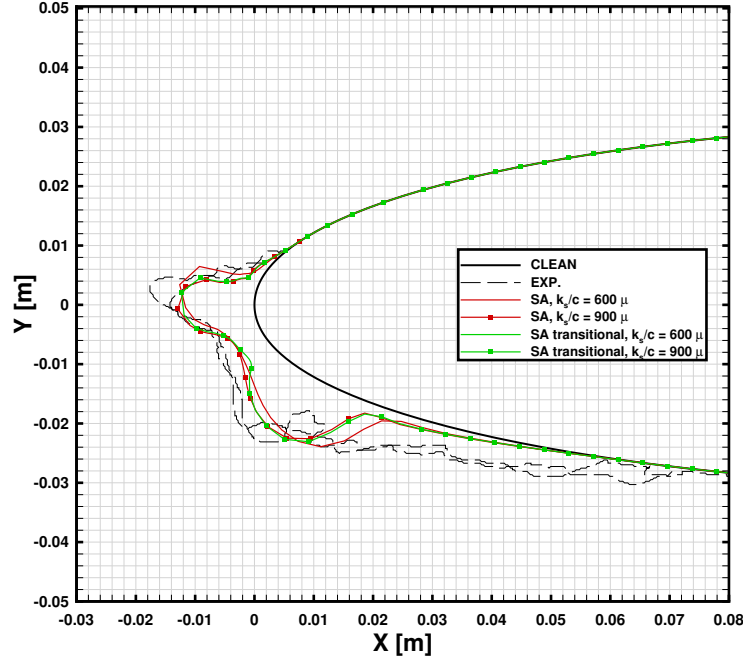


Figure B.4 Ice shapes obtained for NASA IRT case 36 with SA turbulence model and SA- $\gamma\tilde{Re}_{\theta t}$ (SA transitional) transitional model for different global roughness, compared to experimental results (MVD = $20 \mu m$, 6 layers)

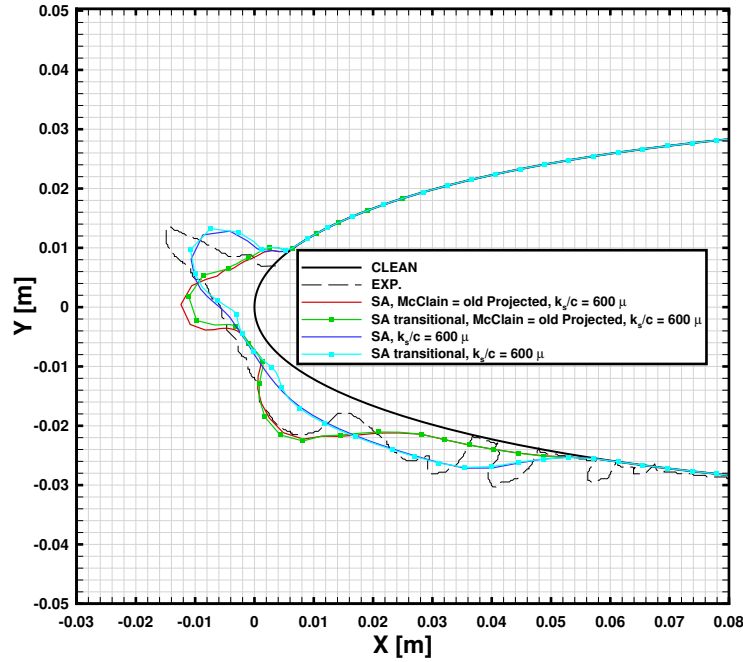


Figure B.5 Ice shapes obtained for NASA IRT case 401 with SA turbulence model and SA- $\gamma\tilde{Re}_{\theta t}$ (SA transitional) transitional model and McClain roughness formulation without the freezing fraction, compared to experimental results (MVD = $20 \mu m$, 4 layers, $k_{s0} = 600 \mu m$)

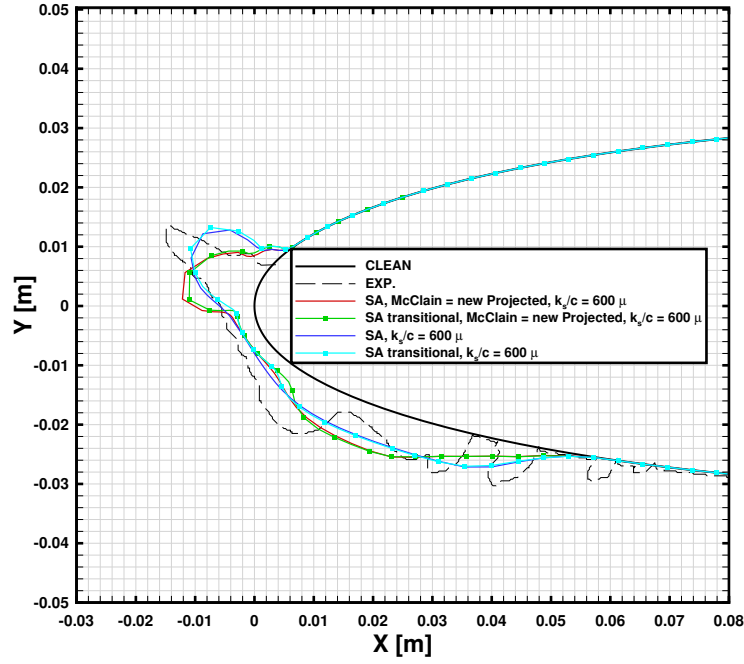


Figure B.6 Ice shapes obtained for NASA IRT case 401 with SA turbulence model and SA- $\gamma\text{-}\tilde{Re}_{\theta t}$ (SA transitional) transitional model and McClain roughness formulation with the freezing fraction, compared to experimental results ($MVD = 20 \mu m$, 4 layers, $k_{s0} = 600 \mu m$)

APPENDIX C HTC RESULTS ON CLEAN SURFACES

This appendix shows additional HTC results, for IRT cases 35 and 36. Different equivalent sand grain roughnesses are applied. The SA turbulence model is employed, with and without the transition extension. The roughness increases in the HTC and laminar regions are observed when a transitional model is used.

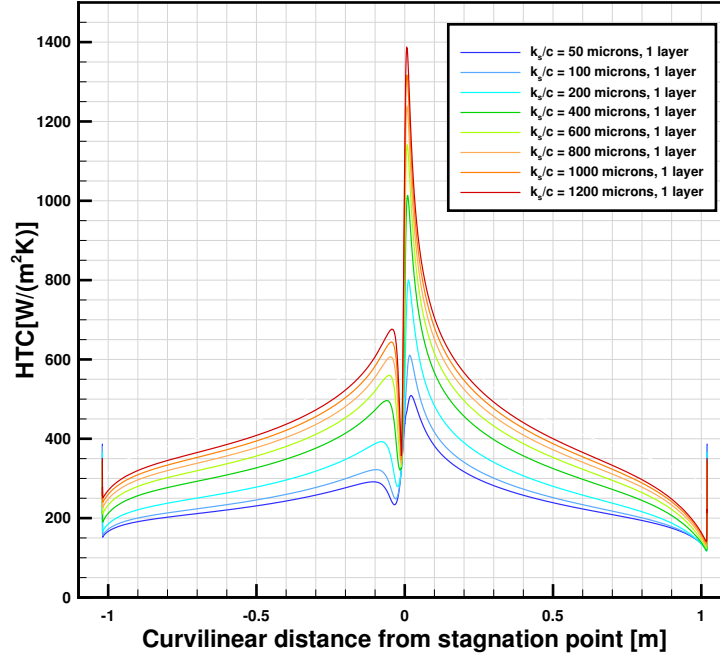


Figure C.1 HTC obtained for NASA IRT case 35 with SA turbulence model and a global roughness formulation ($\text{MVD} = 20 \mu\text{m}$, multiple roughnesses, layer 1)

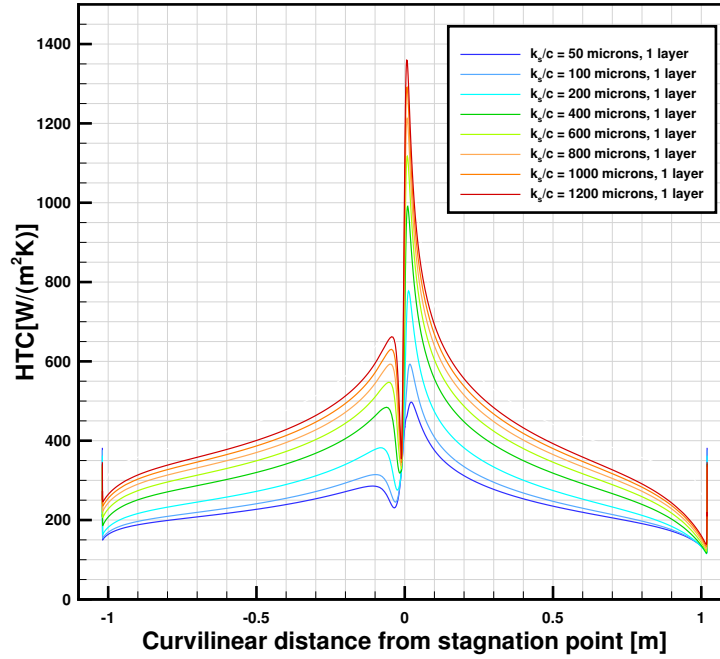


Figure C.2 HTC obtained for NASA IRT case 36 with SA turbulence model and a global roughness formulation ($\text{MVD} = 20 \mu\text{m}$, multiple roughnesses, layer 1)

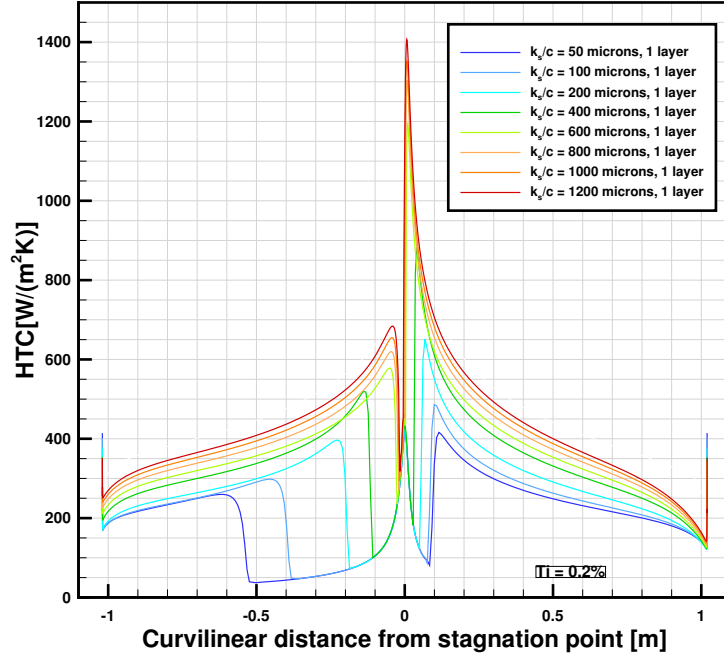


Figure C.3 HTC obtained for NASA IRT case 35 with SA- γ - $\tilde{Re}_{\theta t}$ transitional model and a global roughness formulation (MVD = 20 μm , multiple roughnesses, layer 1)

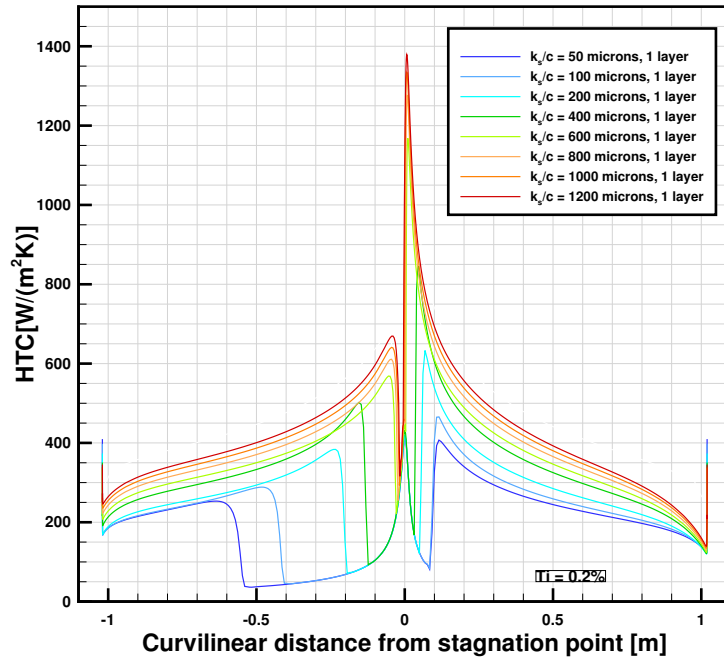


Figure C.4 HTC obtained for NASA IRT case 36 with SA- γ - $\tilde{Re}_{\theta t}$ transitional model and a global roughness formulation (MVD = 20 μm , multiple roughnesses, layer 1)