A COMPUTATIONAL STUDY OF PHASE CHANGE AND MELT TURBULENCE USING PANS MODELLING IN SOLIDIFICATION SYSTEMS

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by

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CERTIFICATE

This is to certify that the thesis entitled "**A Computational Study of Phase Change and Melt Turbulence using PANS Modelling in Solidification Systems**" being submitted by **Mr. Sudeep Verma** is the report of bonafide research work carried by him under my supervision. This thesis has been prepared in conformity with the rules and regulations of Indian Institute of Technology Delhi. I further certify that the thesis has attained a standard required for the award of **Doctor of Philosophy** degree of the Institute. The research reported and the results presented in the thesis have not been submitted, in part or full to any other institute or university for the award of any other degree or diploma.

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(Sudeep Verma)

ABSTRACT

Solidification is a natural phenomenon which is inherent to a number of metallurgical and production engineering processes and technologies which govern a wide range of domain starting from iron and steel industries to the advanced solid-state physics devices. Processes, such as, casting, welding, crystal growth, thermal energy storage are some of the most discernable and key applications of solidification systems. Achieving the desired properties in a final solidified product requires precise control of the transport of mass, momentum and energy in the solidification system. These transport phenomena are governed by the convection in the melt which plays a significant role in controlling the solidification characteristics and quality of the final solidified material. Further the convection in solidification systems may be natural (thermal/solutal buoyancy and surface tension) or forced (external forces due to system rotation, application of electro-magnetic fields, etc.). Moreover, the convective flow in a solidification system can be a slow laminar flow or it can be highly turbulent in the case of welding, casting and Czochralski crystal growth. An accurate modeling of solidification phenomenon in the case of alloy solidification requires an accurate modeling of the thermo-solutal convection in the mushy as well as liquid regions while in processes, such as, Czochralski crystal growth it requires a precise modeling of the melt turbulence.

With the above underlying context, the present thesis deals with exploring some of the above-mentioned issues in different solidification systems. The first solidification system represents a case of a binary alloy solidification governed by strong thermo-solutal buoyant convection in a closed cavity wherein the solid, liquid and mushy zones are modeled using the fixed grid continuum approach. To start with, a detailed comparison is performed amongst the

various mushy zone models for different morphologies of the mushy zone (columnar dendritic and equiaxed) under the aegis of Darcy's porous formulation. Characteristic solidification features of different models in terms of thermal and solutal gradients in the mushy zone, shape and extent of the mushy zone, liquidus front irregularities along with convection in the liquid region and bulk macrosegregation are compared and discussed. Further the buoyancy level in the closed cavity solidification system is also varied from $Ra = 1x10^7$ *to* $Ra = 1x10^9$ *to study the influence of inclusion of important non-Darcian (solid boundary and inertia) effects in the porous formulation of the mushy zone.*

Another solidification system considered in the present thesis is an idealized Czochralski melt flow in an open cylindrical crucible. Controlling the quality of the grown crystals using the Czochralski technique narrows down to controlling the melt convection in the Czochralski melt flow which is highly turbulent due to simultaneous interactions of centrifugal and coriolis forces due to crystal crucible rotations along with buoyancy and surface tension induced forces. The traditional RANS turbulence modeling approach has failed to capture the strong anisotropy and the turbulent time and length statistics in the Czochralski melt flow. Therefore, mainly advanced turbulent modeling approaches, such as, Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS), have been used for tackling turbulence in the Czochralski melt flow. These approaches demand exorbitantly high computational resources. A recently proposed Partially-Averaged Navier-Stokes (PANS) approach has been shown to provide a variable level of resolution from the RANS to DNS based on the filtering of turbulent scales at a comparatively low computational cost. Hence in the present thesis the PANS approach is used for the first time to study the thermo-fluid characteristics of the Czochralski melt flow. Both qualitative and *quantitative comparisons have been performed between the PANS computed results and the reported experimental, LES and DNS results.*

First the variable resolution capability of the PANS approach is demonstrated for the Czochralski melt flow using the PANS low-Re k-ε model. The PANS model at an optimum filter width is shown to capture the important Czochralski flow characteristics in terms of deciphering the melt flow structure, generation of thermal plumes and vortical structures along with capturing the turbulent thermo-fluid characteristics in accordance with the reported experimental, LES and DNS results. Further to gain a thorough physical insight of the Czochralski melt flow, the thermo-fluid dynamics obtained using the PANS variants of the low-Re k-ε and SST k-ω models at an optimum PANS filter width are compared and discussed. The deviations by the models are attributed to the inadequacies of the corresponding parent RANS models. Finally, suitable system rotation and curvature corrections have been applied to both the PANS variants resulting in an improvement in the capabilities of the models in deciphering the true characteristics of the Czochralski melt flow.

सारांश

घनीकरण एक प्राकृतिक प्रक्रिया है जो कई धातुकर्म एवं उत्पादन यांत्रिकी तथा प्रोद्योगिकी प्रक्रियाओ जो की इस्पात उत्पादन से ले कर उच्च तकनिकी ठोसावस्था उपकरणों के विकास को नियंत्रित करती है। कास्टिंग , क्रिस्टल विकास ,थर्मल उर्जा स्टोरेज इत्यादि घनीकरण सिस्टम के कुछ महत्वपूर्ण अनुप्रयोग है। किसी भी घनीकरण उत्पाद मे वांछित गुणों को प्राप्त करने हेतु घनीकरण सिस्टम मे द्रव्यमान, संवेग एवं उर्जा के परिवहन के सटीक नियंत्रण की आव्शयकता होती है। यह परिवहन प्रक्रिया द्रव्य के संवहन पर निर्भर करती है जो की घनीकरण उत्पाद के लक्षणों एवं गुणवत्ता को नियंत्रित करने में महत्वपूर्ण भूमिका निभाता है। इसके अलावा घनीकरण सिस्टम में संवहन प्राकृतिक (थर्मल तथा विलेय उत्प्लावकता और सतह तनाव) या बाहरी (सिस्टम रोटेशन के कारण, इलेक्ट्रो-मैग्नेटिक फील्ड के आवेदन, आदि) से भी हो सकता है। एक घनीकरण सिस्टम में संवहन प्रवाह एक धीमे लैमिनार तरीके से या वेल्डिंग, कास्टिंग और चोक्राल्सकी (Czochralski) क्रिस्टल विकास जैसे सिस्टम मे यह अत्यधिक विक्षोम के साथ हो सकता है। मिश्र धातु के घनीकरण में थर्मल तथा विलेय संवहन की सटीक मॉडलिंग की आवश्यकता होती है, जबकि प्रक्रियाओं, जैसे कि, चोक्राल्सकी क्रिस्टल विकास में द्रव्य विक्षोम के सटीक मॉडलिंग की आवश्यकता होती है।

उपर्युक्त संदर्भ मे प्रस्तुत थीसिस विभिन्न घनीकरण सिस्टम मे उपर्युक्त मुद्दों में से कुछ का अध्ययन करने से संबंधित है। पहला घनीकरण सिस्टम एक बाइनरी मिश्र धातु के घनीकरण का है जिसमे संवहन प्रमुख रूप से थर्मल तथा विलेय उत्प्लावकता द्वारा होता है। इस सिस्टम मे ठोस, तरल और मशी ज़ोन को फिक्स्ड ग्रिड कन्टिन्यूअम एप्रोच का उपयोग करके मॉडल किया गया है। शुरूआत मे विभिन्न मशी ज़ोन मॉडल्स का एक विस्तृत तुलनात्मक अध्ययन प्रस्तुत किय गया है। यह मॉडल्स मुख्यत डार्सी के पोरस मीडियम नियम के आधार पर विकसित है। विभिन्न मॉडलों की विशेषता का आंकलन मशी ज़ोन मे थर्मल तथा विलेय के ग्रैडिएंट्स ,मशी ज़ोन के आकार और सीमा ,लिक्विड फ्रंट की अनियमितता ,तथा तरल क्षेत्र में संवहन के साथ बल्क मैक्रो सैग्रीगेशन के द्वारा किया गया है। तत्पच्यात पहले घनीकरण सिस्टम मे उत्प्लावकता के प्रभाव को Ra = $1x10^7$ से Ra = $1x10^9$ बढ़ा कर महत्वपूर्ण नॉन डार्शियन इफ़ेक्टस (सॉलिड बाउंड्री एवं इनर्शल ड्रैग) के समावेश के प्रभाव का अध्ययन किया गया है।

प्रस्तुत थीसिस मे अध्ययन करने हेतु दूसरा घनीकरण सिस्टम एक आदर्श चोक्राल्सकी क्रिस्टल विकास सिस्टम है। चोक्राल्सकी तकनीक द्वारा उत्पन्न क्रिस्टल की गुणवत्ता मुख्यतः द्रव्य की संवहन पर निर्भर करती है जो कि कई प्रकार के फोर्सेज (थर्मल उत्प्लावकता ,रोटेशनल फोर्सेज और सतह तनाव) के समक्षणिक पारस्परिक प्रभाव के कारण अत्यधिक विक्षोम अवस्था मे होता है। पारंपरिक RANS मॉडलिंग चोक्राल्सकी द्रव्य संवहन की ऐनाइसाट्रपी और विक्षोम को परिकलित करने में विफल रहा है। इसलिए, मुख्य रूप से लार्ज एडी सिमुलेशन (LES) तथा डायरेक्ट न्यूमेरिकल सिमुलेशन (DNS) तकनीको का प्रयोग ही चोक्राल्सकी द्रव्य के विक्षोम के अध्ययन हेतु किया जाता है जो कि अत्यधिक उच्च कम्प्यूटेशनल संसाधनों की मांग करते हैं। हाल ही में प्रस्तावित पार्शिअली अवेरेजड नेवियर-स्टोक्स (PANS) तकनीक ने तुलनात्मक रूप से कम कम्प्यूटेशनल लागत पर RANS से DNS तक द्रव्य विक्षोम का परिकलन करने की क्षमता दर्शायी है। इसलिए इस थीसिस में PANS तकनीक का उपयोग पहली बार चोक्राल्सकी द्रव्य प्रवाह के उष्मीय तथा द्रवीय लक्षणों का अध्ययन करने के लिए किया गया है तथा PANS तकनीक का LES और DNS तकनीको द्वारा परिकलित परिणामों के साथ गुणात्मक और परिमाणात्मक तुलना प्रस्तुत की गयी है।

सर्वप्रथम PANS तकनीक की वेरिएबल रेसोलुशन क्षमता को चोक्राल्सकी द्रव्य प्रवाह मे PANS *low-Re* k-ε मॉडल के द्वारा दर्शाया गया है। तत्पश्चयात PANS मॉडल द्वारा युक्ततम फिल्टर पर चोक्राल्सकी द्रव्य प्रवाह की महत्वपूर्ण प्ररूपी विशेषताओं जैसे की द्रव्य प्रवाह संरचना, थर्मल प्लूम और भंवर संरचनाओं के उत्पादन एवं उष्मीय तथा द्रवीय विक्षोम गुणों को परिकलित कर दिखाया गया है। आगे चोक्राल्सकी द्रव्य प्रवाह की सम्पूर्ण भौतिक जानकारी प्राप्त करने के लिए युक्ततम फिल्टर पर PANS *low-Re* k-ε मॉडल और PANS SST k-ω मॉडल द्वारा परिकलित उष्मीय तथा द्रवीय विशेषताओ की तुलना और चर्चा की गयी है। उपरोक्त PANS मॉडल्स द्वारा परिकलित परिणामो की विसमानताओ का कारण उनके जनक RANS मॉडल्स की अपर्याप्त परिकलित संरचना को दिया जा सकता है जिसे अंतत उपरोक्त PANS मॉडल्स मे रोटेशन तथा स्ट्रीमलाइन कर्वेचर संशोधन द्वारा सुधारा गया है। परिणामस्वरूप उपरोक्त PANS मॉडल्स की परिकलित क्षमता मे सुधार तथा PANS मॉडल्स द्वारा चोक्राल्सकी द्रव्य प्रवाह के सही गुणों तथा लक्षणों का परिकलन होता है।

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NOMENCLATURE

Au	x-momentum source term
Av	y-momentum source term
C_F	form drag constant
C_s and C_l	species concentration in solid and liquid phases of alloy
C_p^s and C_p^l	specific heat of solid and liquid alloy
D	species diffusion coefficient in alloy
D_l	species diffusion coefficient in liquid alloy
e	emissivity
f_k	PANS filter width
f_s and f_l	mass fractions of the solid and liquid phases
g	acceleration due to gravity
g_s and g_l	volume fractions of the solid and liquid phase
Gr	Grashoff (thermal) number
H	crucible height (Solidification system II)
h	sensible enthalpy of the alloy
h_f	latent heat of fusion of alloy
h_s and h_l	sensible enthalpy of solid and liquid phases of alloy
k	turbulent kinetic energy
$\boldsymbol{k}$	permeability
k_0	permeability coefficient
K	thermal conductivity of the alloy
K_s and K_l	thermal conductivities of solid and liquid phases of alloy
k_p	equilibrium partition ratio
L	distance between the hot and cold walls
Ma	Marangoni number
p	effective pressure
Pr	Prandtl number
Ra	Rayleigh number
R_c	crucible radius (Solidification system II)

Re	Reynolds number
Re_w	Reynolds (rotational) number
R_s	crystal radius (Solidification system II)
S_b	buoyancy source term assuming *Boussinesq approximation*
S_h	energy source term
S_C	species source term
S_x	form drag x momentum source term
S_y	form drag y momentum source term
T	temperature
Ta	Taylor number
T_{liq}	liquidus temperature corresponding to solute concentration C
T_m	melting point
$\mathrm{u}(\mathrm{u}, \mathrm{v})$	velocity (x-velocity, y-velocity)
u_l and u_s	solid and liquid velocity

Greek symbols

Δ	average cell dimension
Δi	rate of deformation
Λ	turbulent length scale
α	thermal diffusivity of the alloy
β	coefficient of thermal expansion
β_C	coefficient of solutal expansion
ε	dissipation rate
μ_{eff}	effective viscosity of the liquid
μ_l	dynamic viscosity of the liquid
ρ	alloy/mixture/fluid density
ρ_s and ρ_l	solid and liquid density of alloy
υ	kinematic viscosity of the liquid
τ_s	shear stress due to the surface tension induced forces
ω_c	crucible rotation rate
ω_s	crystal rotation rate
ω	specific dissipation rate

Abbreviation

DNS	Direct numerical simulation
LES	large eddy simulation
PANS	Partially-averaged Navier Stokes
RANS	Reynolds-averaged Navier Stokes
SGS	sub-grid stress