Approximating conditions within a multistage axial compressor and assessing the possibility of hot surface ignition on the heated surfaces

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**NANYANG
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UNIVERSITY**

SINGAPORE

**APPROXIMATING CONDITIONS WITHIN A MULTISTAGE AXIAL
COMPRESSOR AND ASSESSING THE POSSIBILITY OF HOT
SURFACE IGNITION ON THE HEATED SURFACES**

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SCHOOL OF MECHANICAL AND AEROSPACE ENGINEERING

2018

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COMPRESSOR AND ASSESSING THE POSSIBILITY OF HOT
SURFACE IGNITION ON THE HEATED SURFACES**

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Summary

Aero-derivative gas turbines are deployed on offshore oil and gas production platforms, among other engine types and locations relevant to the industry. These gas turbines continuously ingest large amounts of air from their surroundings, presenting the possibility that leaking flammable gas may be drawn into the air intakes and the gas turbine ingests the leaking flammable gas. When leaking flammable gas is detected on a platform, gas turbines initiate wind down by rapidly turning off their fuel supply. As the gas turbine winds down, the ingested flammable gas and air arrives at the last stages of the compressor. The mixture of flammable gas and air is now slowing down over and being heated by the hot internal surfaces found at the rear of the compressor and subsequently in the combustor and in the turbine. The present study develops a stage un-stacking method that approximates the conditions within the multistage axial compressor of a gas turbine. Under the conditions approximated above, the present study continues to examine the possibility of hot surface ignition taking place on the heated surfaces within the compressor.

After unstacking the axial compressor of the LM2500 aero-derivative gas turbine, only the last 2 stages attain a mean temperature of about 680 K and 723 K respectively. On the heated surfaces, a 2-step reaction mechanism for methane and oxygen implemented with finite rate chemistry, numerically models the reaction between methane gas and oxygen. The Van't Hoff ignition criterion indicates ignition on the surface when the local temperature gradient crosses zero. The chemistry model is validated using the Smyth and Bryner [1]

experiment and achieves acceptable agreement with an ignition temperature between 1300 K and 1310 K (compared to 1252 K to 1367 K) for low speed flow at about 0.16 m s^{-1} . The temperature difference between the normally operating axial compressor and ignition temperature is at least 577 K. Given forced convection flows within the axial compressor during wind down, the metal surfaces will cool down and the required ignition temperature will rise. The temperature difference to overcome for ignition will widen. The probability that an ignition scenario develops into a hot surface ignition is considered very low.

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Nomenclature

Symbols with more than 1 meaning are grouped together.

Upper case

A	Turbomachinery station cross sectional area (m^2) Pre-exponent for the Arrhenius rate equation (units depending on species concentration exponent) Area (m^2)
B	Fraction of unblocked cross sectional area (dimensionless) Pre-exponent for ignition time delay (units depending on species concentration exponent)
C	Fuel concentration exponent (dimensionless)
C_F	Coefficient of fluid resistance for a turning rotor
D	Oxidiser concentration exponent (dimensionless) Diffusion Factor, a measure of the blade loading (dimensionless)
D_{CH_4}	Effective diffusion coefficient of CH_4 into the bulk species ($\text{m}^2 \text{s}^{-1}$)
D_{Im}	The effective diffusion coefficient of species I into bulk species m ($\text{m}^2 \text{s}^{-1}$)
E_a	Activation energy (J kg^{-1})
F_1, F_2	Blending functions in k - ω turbulence model (dimensionless)
HR	Heat rate (dimensionless)
$\mathbf{I}$	Unit tensor (dimensionless)
I	Elements of the Unit tensor (dimensionless)
I	The index to denote individual chemical species (dimensionless)
I_{TURB}	Turbulence intensity (dimensionless)
I_M	Moment of inertia
J	Mechanical equivalent of heat, 778.2 ft-lb/Btu or 1 J/J where 1 ft-lb=1.35582 J and 1 Btu = 1055.06 J (dimensionless)
$\vec{J}_I$	The flux of the I^{th} species ($\text{kg m}^{-2} \text{s}^{-1}$)
Ka	Karlovitz number (dimensionless)

LHV	Lower heating value (J kg^{-1})
M	Molar Mass of a chemical species (kg mol^{-1}) Third body in termolecular reactions (no dimensions)
N	The number of chemical species (dimensionless)
N_{AV}	Avogadro's number (dimensionless)
N_B	Number of blades in a blade row (dimensionless)
OPR	Overall pressure ratio of the compressor (dimensionless)
P	Absolute static pressure (Pa)
P_k	Production of turbulent kinetic energy ($\text{m}^2 \text{s}^{-3}$)
P_ω	Production of Turbulent eddy frequency or specific turbulence dissipation ($\text{m}^2 \text{s}^{-2}$)
Pr	Prandtl Number (Pa)
PR_{MOD}	Stage pressure ratio determined from the pressure ratio models (dimensionless)
PR_{ACT}	Actual stage pressure ratio used (dimensionless)
$P(\)$	Probability (dimensionless)
R	Gas constant for air ($\text{J kg}^{-1} \text{K}^{-1}$)
R_{V,CH_4}	Volumetric production rate of CH_4 (mol m^{-3})
R_{REACT}	Stage degree of reaction (dimensionless)
Re	Reynolds number (dimensionless)
S	An invariant measure of the strain rate (s^{-1})
S^c	Source term for reaction progress variable (dimensionless)
S_M	External momentum sources ($\text{kg m}^{-2} \text{s}^{-2}$)
S_E	External energy sources ($\text{J m}^3 \text{s}^{-1}$)
S_{Y_I}	Sources for Y_I changes for the I^{th} chemical species ($\text{kg m}^3 \text{s}^{-1}$)
T	Absolute Temperature (K)

T_{FOIL}	Foil surface temperature (K)
T_{MAX}	Maximum domain temperature after ignition (K)
T_0	The reference temperature (K)
U_{∞}	Free stream speed (m s^{-1})
$\vec{U}_{\text{WHEEL}}$	The rotor tangential speed, also referred to as wheel speed U_{WHEEL} (m s^{-1})
$\vec{V}_{\text{ABS}}$	The absolute velocity in the velocity triangles for turbo-machinery analysis and also referred to as V_{ABS} (m s^{-1})
$\vec{V}_{\text{REL}}$	The free stream velocity outside the boundary layer, which is the velocity relative to the blade which is the relative velocity in the velocity triangle analysis for turbo-machinery and also referred to as V_{REL} (m s^{-1})
V_{DS}	The general symbol for a design variable (depends on variable)
W_{OUT}	Gas turbine work output (J kg^{-1})
Y_I	The mass fraction for the I^{th} species (dimensionless)

Lower case

a_1	Coefficient of proportionality for shear stress in a boundary layer to the turbulent kinetic energy (dimensionless)
$\vec{b}^s$	Row vector which is a dual basis vector for the slow reactions for $\frac{\partial}{\partial t} \vec{y}$ in the CSP method (dimensionless)
c	Chord of an airfoil (dimensionless) Reaction progress variable (dimensionless)
c_p	Specific heat capacity at constant pressure ($\text{J kg}^{-1} \text{K}^{-1}$)
c_v	Specific heat capacity at constant volume ($\text{J kg}^{-1} \text{K}^{-1}$)
d	Diameter (m)
d_{CH_4}	Molecular diameter of a methane molecule (m)
d_{HYD}	Hydraulic diameter (m)

d_{O_2}	Molecular diameter of an oxygen molecule (m)
e	Specific internal energy (J kg ⁻¹)
e_{ij}	Strain rate tensor (s ⁻¹)
e_{WHIRL}	Euler whirl (J kg ⁻¹)
f	Symbol for a general quantity (units depending on the analysis)
f_{RELAX}	The general symbol for a relaxation factor (dimensionless)
$\vec{g}$	Gravitational acceleration or the gradient of gravitational potential (m s ⁻²)
h	Specific enthalpy (J kg ⁻¹)
h_I	Specific enthalpy of the I^{th} species (J kg ⁻¹)
Δh_{COMB}	Energy released in combustion per unit of fuel (J mol ⁻¹)
$\Delta h_{f,I}^0$	Specific enthalpy of formation for chemical species I (J kg ⁻¹)
Δh_{REACT}	Energy absorbed in a reaction per unit of reactant (J mol ⁻¹)
i	An index for tensor notation when in subscript (dimensionless) Time step number (dimensionless)
j	An index for tensor notation when in subscript (dimensionless)
k	Turbulent kinetic energy (m ² s ⁻²) An index for tensor notation when in subscript (dimensionless)
k_{AMB}	The initial ambient k (m ² s ⁻²)
k_{BM}	Boltzmann constant (m ² kg s ⁻² K ⁻¹)
k_{LOSS}	The coefficient of loss for flow in the Bernoulli equation (dimensionless)
k_{PR}	Fraction of the actual of the stage pressure ratio to the maximum possible stage pressure ratio found in the pressure ratio models (dimensionless)
$k_{PR,1}$	The k_{PR} for stage 1 of the compressor (dimensionless)
k_u	The fraction of wheel speed at the OGV inlet (dimensionless)
m	The index for bulk species (dimensionless)

	An index in tensor notation when in subscript (dimensionless)
	Mass (kg)
m_I	The mass of the I^{th} species (kg)
$\dot{m}$	Mass flow rate (kg s^{-1})
n	Spatial coordinate normal to the surface (m), Exponent of u' in turbulent flame speed correlations (dimensionless), Exponent of ω in rotating component wind down
q	Heat flux across the boundaries of the control volume ($\text{J m}^{-2} \text{s}^{-1}$)
$\dot{q}_{\text{RAD}}$	Rate of change of energy due to radiation (J s^{-1})
r_{CASE}	Casing radius (m)
r_{CORE}	Hub radius (m)
r_E	Eulerian radius (m)
Δr	Annulus gap (m)
s	Specific entropy ($\text{J kg}^{-1} \text{K}^{-1}$) Number of CSP reactions (dimensionless)
s_f	The volumetric source from outside the control volume (units depending on the analysis)
s_0	Specific reference entropy from thermodynamic tables ($\text{J kg}^{-1} \text{K}^{-1}$)
t	Time (s)
Δt	Time step (s)
$t_{1\text{ST,IGN}}$	Time to 1 st ignition (s)
$\vec{u}$ or u_i	Velocity vector (m s^{-1})
u, v, w	Velocity magnitude in the x, y, z axes respectively (m s^{-1})
$\vec{u}$ or u	Axial component in turbomachinery of $\vec{V}_{\text{ABS}}$ also referred to as u (m s^{-1})
$\bar{u}$	Mean velocity (m s^{-1})
u'	Instantaneous velocity fluctuation (m s^{-1})

$\vec{v}$ or v	Tangential component in turbomachinery of $\vec{V}_{ABS}$ also referred to as v (m s^{-1}),
$\vec{x}$ or x_i	Position vector (m)
x	Axial coordinate of the compressor in turbomachinery (m)
x, y, z	Cartesian coordinates (m)
y_{NW}	The distance to nearest wall in the blending functions (m)
$\vec{y}$	Column vector of chemical species mass fractions (dimensionless)
$\vec{y}^R$	Column vector containing the net production each species

Greek

α	The flow angle of the $\vec{V}_{ABS}$ makes with the axial direction in velocity triangle analysis for turbo-machinery (°)
$\alpha_1, \alpha_2, \alpha_3$	Coefficients in the k - ω turbulence model (dimensionless)
β	The flow angle of the $\vec{V}_{REL}$ makes with the axial direction in velocity triangle analysis for turbo-machinery (°)
$\beta_1, \beta_2, \beta_3$	Coefficients in the k - ω turbulence model (dimensionless)
β'	Coefficient in the baseline k - ω turbulence model (dimensionless)
γ	The ratio of specific heats, c_P/c_V (dimensionless)
$\bar{\gamma}$	Mean ratio of specific heats between two or more stations in the compressor (dimensionless)
ε	A general symbol for an error variable in iteration (dimensionless) Turbulence dissipation ($\text{m}^2 \text{s}^{-3}$)
η	Thermodynamic efficiency (dimensionless)
$\vec{\eta}^S$	CSP vector with elements η^S (dimensionless)
θ_{ROT}	The angle of the curvature of the rotor blade (°)
θ_{STA}	The angle of the curvature of the stator blade (°)
$\Delta\theta$	The difference in angle of curvature of the rotor and stator (°)

κ	Thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)
μ	Dynamic viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
μ_{TURB}	Turbulence viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
μ_{RM}	Reduced mass (kg)
ν	Kinematic viscosity ($\text{m}^2 \text{s}^{-1}$)
ρ	Density of the working fluid usually air (kg m^{-3})
σ	Blade solidity which is the ratio of chord to pitch (dimensionless)
σ_{CS}	Collision cross section (m^2)
$\sigma_{k1}, \sigma_{k2}, \sigma_{k3}$	Coefficients in the k - ω turbulence model (dimensionless)
$\sigma_{\omega1}, \sigma_{\omega2}, \sigma_{\omega3}$	Coefficients in the k - ω turbulence model (dimensionless)
σ_f	The volumetric source from within the control volume (units depending on the analysis)
τ	Viscous stress tensor ($\text{kg m}^{-1} \text{s}^{-2}$)
τ_{IGN}	Ignition time delay (s)
ϕ_f	The flux across the control volume surface (units depending on the analysis)
ψ	Gravitational potential ($\text{m}^2 \text{s}^{-2}$) The Stage Load Coefficient (dimensionless)
ψ_{DS}	The design SLC, which could be a single value for all stages or a distribution of values by stage (dimensionless)
ω	Shaft rotational speed (rad s^{-1}) Turbulent eddy frequency or specific turbulence dissipation (s^{-1})
ω_{AMB}	The ambient ω set as the initial ambient ω (s^{-1})

Subscripts

0	Reference conditions
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1	The blade leading edge which is also considered to be equivalent to the upstream measuring station of the blade row or blade row inlet station
2	The blade trailing edge which is considered to be equivalent to the downstream measuring station of the blade row or blade row outlet station
ABS	Absolute
ALT	Alternative
AMB	Ambient
APP	Approximate
AV	Avogadro
BM	Boltzmann
BUO	Buoyancy
BWD	Backward
CASE	The compressor casing
CFD	Computational fluid dynamics
COMB	Combustion
COMP	full compressor
CONC	Concentration
CORE	The compressor hub
CS	Cross section
Corr	Corrected value
DS	Design
EQM	Equilibrium
EXT	Extra or additional Extrapolate for time step or grid refinement
FWD	Forward
GAP	Annulus gap

HARD	Strict or fixed conditions or criteria
HYD	Hydraulic
IGN	Ignition
IGV	Inlet guide vanes
IN	The stage inlet station
INIT	Initial
MAX	Maximum value of a variable
mean	Mean value
MIN	Minimum value of a variable
NEW	Updated values of a design variable
OLD	Previous values of a design variable
OUT	The stage outlet station
POLY	Polytrophic
PRO	Progress
REACT	Reaction
REL	Relative to the blade
RM	Reduced mass
ROT	Rotor
SOFT	Less strict or flexible conditions or criteria
STA	Stator
STG	Stage
SURF	Surface
SUSM	Stage un-stacking method
TOT	Total or stagnation properties
TURB	Turbulence

(g) Gaseous state of the chemical species

i Isentropic condition

Script

$d\mathcal{H}$ The de Haller number (dimensionless)

ℓ Length in Reynolds number (m)

Superscripts

EQM Equilibrium

UB Unburnt

Chapter 1. INTRODUCTION

During the time of the present study, the search for oil and gas has extended to remote offshore locations. On the Norwegian continental shelf, exploration has reached middle of the North Sea. Not far away, there are also plans for exploration on the Barents Sea.

Oil and gas extraction is a technologically intensive process using various forms of energy. Electrical energy powers for electric motors, instruments and computers. Mechanical energy supports gas compression before sending gas into pipelines for onshore for processing.

1.1 Background

At offshore locations, diesel engines and gas turbines are commonly deployed on-site to provide generator drive and mechanical drive.

Diesel engines were driving the electrical generators for the Deepwater Horizon [2] semi-submersible. The Deepwater Horizon incident shows clearly that a major accident of this scale requires continuous electrical power generation to operate the necessary firefighting systems [3]. To supply continuous electrical power, even during a gas leak event, the ideal engine would pose no explosion or fire risk should the engine be ingesting flammable gas with air.

The gas turbine is generally more efficient for mechanical drive applications requiring constant speed. Being a complex piece of equipment, separating the gas turbine into simpler components for explosion-proof testing is not feasible. To date the risk of ignition posed by a gas turbine operating in a flammable gas environment on an offshore oil and gas platform is uncertain.

1.2 Research motivation

Oil and gas extraction and production platforms are compact facilities, with a high number of process equipment found within a small volume of space. While in operation, gas leaks that do occur in oil and gas facilities expose the process equipment to the flammable gases. A typical quantitative risk analysis performed for offshore oil and gas platform in the North Sea would consider the probability of flammable gas exposure to ignition sources, $P(exposure)$ and the probability of ignition when flammable gas is exposed to an ignition source, $P(ignition | exposure)$ as seen in Equation (1.1), taken from [4].

$$P(ignition) = P(exposure) \times P(ignition | exposure) \quad (1.1)$$

The final probability of ignition, according to Equation (1.1) is the probability of ignition of flammable gas by equipment used on an offshore oil and gas platform.

A study into leak and ignition events in the North Sea is carried out by Lloyd's Register Consulting and Lilleaker for the Norwegian Oil and Gas association in 2013 [4] and updated in 2017 [5]. Among other ignition sources, the gas turbine is identified as a likely source of ignition in the few major leak and ignition events. The study concluded by emphasizing the need to study the probability

of ignition from a gas turbine to realise greater safety levels for the oil and gas industry on the Norwegian continental shelf.

The gas turbine ingests huge quantities of air from the surroundings as the working fluid. When flammable gas leaks, this air is contaminated, the gas detection system will trigger and eventually the gas turbine winds down. In the latter half of the wind down process, the possibility of hot metallic surfaces in contact with the low-speed air and gas mixture poses a potential increase in probability of ignition. This potentially affects the ignition probabilities used in quantitative risk analyses, resulting in greater anticipated explosion loads on the structures, which in turn affect the overall design for safety.

Through harnessing the prevailing winds and using a well-ventilated or porous platform construction, flammable gas leaks would not accumulate but instead be swept downstream. In parallel, the air intakes of the gas turbine are located away from the downstream path of the prevailing winds. These factors greatly reduce the probability of leaking flammable gas finding its way directly to and into the air intakes of the gas turbine.

A possible incident scenario would consist of a still day with no prevailing wind blowing or a slight wind blowing in the reverse direction of the prevailing winds. This allows leaked gases to accumulate or even move towards the unintended parts of the platform, where local convection and turbulent flow are actively mixing and diluting the leaked gas. The gas detection system will trigger an alarm for leaked gas. During wind down, the gas turbine air intakes cannot shut

out air from the external environment as the high-pressure spool must be turning at a minimum rotational speed to continually drawing air in until the temperature becomes sufficiently low, a process that prevents bowing of the high-pressure spool shaft.

Methane is the majority species in natural gas so it is used to represent the leaked natural gas. With the typical leak rates in Table 3.2 of Pedersen [6], and at normal temperature and pressure conditions (NTP), 293.15 K and 101325 Pa, the resulting concentration levels of methane are usually much lower than the lower flammability limit (LFL). Equivalence ratio in the present study is the ratio of the actual molar ratio of methane to air compared to the stoichiometric molar ratio of methane to air. To maintain an equivalence ratio of 1.0 from a methane gas leak at 10 kg s^{-1} , the resulting mixture of air and methane contains 6604.9 moles. This amount of air and methane must fill up a volume of 158.88 m^3 each second, in other words an equivalent cube of edge 5.416 m is filled every second at NTP. At smaller leak rates, the volume of air that maintains the equivalence ratio at 1.0 is shown in Table 1.1. It is likely a leak rate at 10 kg s^{-1} escapes forcefully, is not contained and mixes with much more air, resulting in lower equivalence ratios.

Table 1.1. Leak rates and approximate volume of resulting methane-air mixture at equivalence ratio 1.0

Leak rate [kg s^{-1}]	Leak rate [mol s^{-1}]	Resulting mixture amount at equivalence ratio 1.0 [mol]	Volume of mixture [m^3]	Edge of equivalent cube [m]
0.1	6.2334	66.049	1.589	1.169
1.0	62.334	660.49	15.89	2.514
10.0	623.34	6604.9	158.9	5.416

The following 2 assumptions are made.

- A1 The reliability of the gas detection system as a whole is 100%, though the individual sensors need not perform perfectly. The gas detection system will sense a gas leak, should there be one and without ambiguity or delay, send this signal to the gas turbine control system.
- A2 The reliability of the gas turbine control system (residing on the gas turbine or on the package for the gas turbine) is 100%, fully capable of shutting off the fuel supply and executing the required wind down procedure.

A range of 9 possible ignition scenarios (referred to as IGS-1 through IGS-9 in the present study) is studied by Pedersen [6].

In IGS-1, at methane concentration, $[CH_4] < 20\%$ of LFL, no ignition is possible. However, as temperature and pressure increases, flammability limits generally widen by lowering the LFL concentration and increasing the UFL concentration. [7] For operating air breathing machines, especially engines, in an oil and gas context, there is unlikely a design limit or statutory limit imposed on the highest temperature and pressure that may be harnessed by these machines. Considering that the LFL reduces as temperature or pressure increase, it would not be immediately clear what this ignition-safe minimum concentration implies.

In IGS-2, IGS-4 and IGS-8, Pedersen [6] covers the full range of concentrations under the scenario that detection of leaked gas is unsuccessful. This strongly complicates the study as the failure mode of another device is considered. The

implication of no detection is that the gas turbine is able to continue functioning, in normal or degraded mode, ingesting methane and air instead of clean air. This concern is also addressed in all the other ignition scenarios IGS-3, IGS-5, IGS-6, IGS-7, IGS-9 where gas detection takes place.

In IGS-3, IGS-5, IGS-6, IGS-7 and IGS-9, these ignition scenarios do not involve any failure mode of any other device as gas detection is successful and the gas turbine winds down according to design. However, this wind down process is not immediate. While the response time of the gas detection system and gas turbine control system is very short, this is not an indication that eventually no gas reaches inside the gas turbine before the gas turbine shuts down. Since methane may reach into the gas turbine, the possibility that the gas turbine is able to continue functioning, ingesting methane and air is addressed in the present study as a phase of operation before the wind down procedure starts. IGS-5 is extended with a time factor in IGS-6 and IGS-7. As mentioned above, the flammability limits widen in both directions as pressure or temperature rises [7]. Setting up IGS-5, IGS-6 and IGS-7 based on LFL and UFL at NTP or at similar conditions artificially narrows the range of methane concentration that may pose an ignition problem.

Streamlining the simulation effort, the following few scenarios (SS) are considered in greater depth.

SS1 The gas turbine ingests methane gas while running and before shut down

Wind down will occur as the 2 systems mentioned in the assumptions A1 and A2 work as intended. The combustor section is the hottest and the on-going combustion will ignite the methane gas. This takes place near and outside the primary zone of the combustor. The ignition of ingested methane gas, which is fuel not entering the combustor via the fuel system, but taking place inside the primary zone or secondary zone of a combustor does not pose an operation problem to the combustor because combustion is meant to take place in the primary and secondary zones. The effect of ingested methane gas is simply more fuel that increases turbine inlet temperature and shaft rotational speed, events that will eventually signal a wind down. Before the gas turbine winds down, the ingested methane leads to 2 different possibilities:

SS1.1 Damage to the combustor liner

The combustor liner may be conceived as a sheet of oxidation resistant (Hastelloy X and Haynes 188 [8]) metal alloy, punctured and perforated with holes at strategic locations to guide the flow of compressed air to set up the vortex flow structures in the primary and secondary zone and to provide a layer of cooler air that protects the liner via film cooling.

The combustor liner may be damaged in 2 ways, a) when the flame in the primary zone expands beyond the space intended for it and touches the liner and b) a flame may start within the layer of film cooling air.

Air that supports combustion in the primary zone should contain no more than a small fraction of a percent of residual flammable gas entrained in the air. The detail of increased concentration of ingested methane that supports flame expansion out of the primary zone is not part of the present study.

The film cooling air contains methane and has a low flow speed due to the walls of the combustor liner. The concentration range of methane and the speed below which burning is supported within the layer of cooling air is not part of the present study.

Suppose a perfect storm occurs where the complete breakdown of the combustor liner materializes. The damaged combustor liner will severely impede setting up the correct vortex structures, rendering the combustor less effective as seen in the great amount of detail that Mattingly et al. [9] and Jones [10] point out that goes into setting up the correct vortex structures. It is possible that combustion might cease all together but probably not before damage is done when the turbine over speeds for that short duration. The duration of the window of over speeding is defined by the response time of the gas detection system to signal a wind down, the response time of the fuel system to fully shutoff the fuel valve(s), the remaining fuel to be consumed and the last contribution to this window is the amount of ingested methane.

The mechanism of sustaining damage through over speeding is not part of the present study.

SS1.2 Possibility of flames propagating upstream against the compressor flow and emerging from the compressor front

The conditions in the compressor may or may not support combustion since speeds are above 137 m s^{-1} [11]. The turbulent intensity is generally high and likely to be above 10%, therefore u' is at least $\pm 13 \text{ m s}^{-1}$. The highest possible laminar burning velocity for methane is about 0.37 m s^{-1} at an equivalence ratio of 1.05, read off from Figure 6 in Bibrzycki and Poinso [12]. Flame acceleration due to turbulence generally scales with u'^n . Chaudhuri et al. [13] experimentally determine $n = 0.5$. Before that, Gerdner et al. [14] experimentally determine $n = 0.27$. Invoking the theoretical flame quenching condition of Karlovitz number $Ka > 1$ and using the Ka correlation in Equation (4) of [14], Gerdner et al. sets the maximum u' which in turn determines the maximum turbulent flame acceleration before quenching takes place. A number of feasible turbulent flame acceleration correlations exist however they are not paired with a corresponding Ka correlation that involves u' in the range $Ka \leq 1$. Without a known maximum u' , the maximum turbulent flame speed cannot be compared to the turbulent velocity fluctuations.

While still running in the narrow window of time before wind down, the ingested methane gas encounters increasing pressure and temperatures going through the compressor. While these 2 factors increase reaction rate, their effects are not directly clear. The possibility that the flame of combustion could be travelling against the flow in the compressor, together with effect of increasing pressure and temperatures on the reaction rate is further analysed.

When the wind down signal is received, inevitably the fuel system shuts the fuel supply and the gas turbine will wind down. For the gas turbine to continue running without fuel and without other controls such as bleed valves, variable guide vanes, engine control (for example, the Full Authority Digital Engine Control, or FADEC), the flow at design operating point must be maintained such that variable stator actuation is not required. The gas turbine would require the same fuel flow rate to be supplied by ingested methane. This is highly unlikely as the required fuel concentration is too high, as leaked gas needs to enter the gas turbine to supply energy equivalent to 1.4 kg s^{-1} of fuel to replace the fuel flow rate. This fuel flow rate is reported in Pedersen [6]. This is highly unlikely to be maintained at a consistent level by the leaked gas and air outside as the leak must be much larger and cannot be subject to the randomness of turbulent convective flows in the open. Eventually, without deliberate intelligent control of the other supporting functions, the gas turbine will wind down.

SS2 Gas turbine ingests methane gas while winding down

As the gas turbine is an air breathing engine, it does not shut off the air supply. The pre-defined wind down procedure calls for a duration of turning the high pressure spool at a specific rotational speed to reduce shaft bowing during cooling and improve cooling so that the gas turbine cools sooner and the next start-up may start earlier. During the wind down, the hot surfaces are always exposed to methane gas.

At any part, the gas turbine is hottest at the start of wind down. During wind down, all three quantities pressure, temperature and speed dissipate together. Depending on the design of the wind down profile, a number of possibilities exist. Pressure reduces the fastest and temperature reduces the slowest according to Pedersen [15] for the LM2500 by General Electric.

The parameter space of temperature, pressure and speed (alternatively rotational speed or mass flow rate) seen in the gas turbine in the present study is shown in Figure 1.1. The subscripts “DS” refer to design operating point and “REST” refer to complete wind down with residual mass flow rate drifting through the gas turbine due to convection at the exhaust stacks. The 8 possible combinations are found at the 8 corners of the cube in this parameter space.

The combinations of conditions suitable for simulation are indicated as case 1 and case 4. The scenario SS1.2 before wind down translates to simulation case

1, where the gas turbine is running normally and the compressor outlet is at conditions T_3 , P_3 and $\dot{m}_{DS}$. The scenario SS2 translates to simulation case 4, where the gas turbine has commenced wind down except the compressor outlet is maintained at an artificially high temperature T_3 , while the other conditions are P_1 and $\dot{m}_{REST}$.

$$\begin{aligned} P_1 &= 101325 \text{ [Pa]} \\ T_1 &= 278.15 \text{ [K]} \\ n_{GG.REST} &= 0 \text{ [RPM]} \\ \dot{m}_{REST} &= 3.0 \text{ [kg/s]} \end{aligned}$$

$$\begin{aligned} P_3 &= 1819000 \text{ [Pa]} \\ T_3 &= 723.45 \text{ [K]} \\ n_{GG.DS} &= 9424 \text{ [RPM]} \\ \dot{m}_{DS} &= 68.2 \text{ [kg/s]} \end{aligned}$$

Figure 1.1. Compressor temperature, pressure and mass flow rate changes during a LM2500 gas turbine wind down

The simulation case 4 may be further translated into a simulation of slow flow at ambient pressure through a heated duct. To analyse case 4, the 2 most relevant sets of experimental data to the author's knowledge are the experiments of Robinson and Smith [16] and Smyth and Bryner [1]. For a stagnant methane-air mixture heated by a stainless steel surface, the experimental outcomes from Robinson and Smith [16], reproduced in Figure 1.2, point to a minimum auto-ignition temperature of 884 K occurring at equivalence

ratio 0.7. (Legend details: square, 0 m/s, “SS” for stainless steel and “RS” for Robinson and Smith.)

Figure 1.2. Experimentally determined auto ignition temperature for methane-air mixtures from Robinson and Smith [16] and Smyth and Bryner [1]

For methane-air mixtures, flowing over a heated metallic surface, Smyth and Bryner [1], reported auto-ignition temperatures in the range 1252 K to 1367 K (Figure 1.2) for 3 metallic surfaces occurring at equivalence ratio 0.7. (Legend details: triangle-cross-circle, 0.16 m/s for inlet flow speed, “SS” for stainless steel, “Ni” for nickel and “Ti” for Titanium and “SB” for Smyth and Bryner.)

Simulation case 4, in a possible worst scenario, would consist of metallic surfaces of the last axial compressor stage at 723.45 K [6], the momentum of the high-pressure spool artificially dissipating rapidly resulting in almost stationary air and a mixture of methane and air at equivalence ratio 0.7 flowing through. This puts the flow field, temperature field of the simplified wind down

scenario about 160 K below that found in the experiment of Robinson and Smith [16]. Since ignition occurred in the experiment of Robinson and Smith [16], it is productive to investigate the possibility of ignition in the conditions inside the last compressor stage, especially when flow velocities go down to zero and temperatures remain high enough. Increased clarity on the temperature and velocity relation to ignition by hot surfaces potentially improves risk analyses.

1.3 Hypothesis

The scenario of a gas turbine ingesting flammable gas from a gas leak on an offshore oil and gas platform may be efficiently analysed by developing a multistage axial compressor model and a hot surface ignition model. These support determining probability of ignition given exposure, where a running gas turbine ingests methane gas and when the same gas turbine completely winds down.

1.4 Objectives

The objectives of the present study are

1. Develop a method to approximate the conditions within the multistage axial compressor of a gas turbine.
2. Under the conditions approximated above, examine the possibility of hot surface ignition taking place on the heated surfaces within the compressor.

1.5 Scope

The specific gas turbine used in the present study is the LM2500 by General Electric, a common model on the Norwegian continental shelf. The gas turbine is deployed on an offshore platform together with gas production facilities. The gas detectors are generally very reliable and used in groups, allowing the reasonable assumption that gas detection is certain. This study considers the unfortunate scenario where leaking flammable gas does not to disperse away from the gas turbine air intakes as intended and leaking flammable gas passes into the air intakes. This gives rise to a scenario that the gas turbine could be running at the first instance of ingesting gas or shutting down at the first instance of ingesting gas. Therefore, within the present study $P(exposure) = 1.0$. The 2 specific scenarios considered in the present study are gas ingested by a gas turbine running normally and gas ingested by gas turbine that has shut down but temperatures remains as high as during normal running.

The flow in only the primary flow path of the axial compressor is studied. The thermodynamic analysis, axial variation analysis and velocity triangle analysis is carried out for the axial compressor operating at its design operating point. A reasonable distribution of stage loading coefficients is sought for the entire compressor. At each stage, the axial velocity together with the Euler whirl equation sets up the stage velocity triangles. Majority of the calculations are iterative. Eventually, the stage-to-stage variation of temperature, pressure, flow speed and flow angles is approximated. Knowing this, analysis can now focus on the temperature and velocity profiles of the last two stages of the LM2500

axial compressor, since the temperatures here are about 160 K below the lowest reported auto ignition temperature of methane gas.

To consider the hot surface ignition possibility, a finite rate implementation of a simpler 2-step reaction mechanism by Westbrook and Dryer [17] for methane combustion in air is first numerically validated against the experimental outcomes of Smyth and Bryner [1]. The Arrhenius rate equation sets the reaction rate. The Van't Hoff ignition criterion indicates ignition on the heated surface when the immediate pocket of gas on the surface attains the same temperature as the surface. This validated chemistry model is then applied to the flow conditions found within the last 2 stages of the LM2500 axial compressor and conclusions are drawn about the possibilities of hot surface ignition when methane is ingested by a normally running gas turbine and by gas turbine that has wound down but temperatures remains as high as during normal running.

1.6 Contributions

The present study contributes the following:

1. A stage un-stacking method is developed to realistically estimate the temperature, pressure, flow angles and flow velocities at each stage of an axial compressor for in-service gas turbines. The method uses information that non original-equipment-manufacturers commonly access, reducing reliance on the original-equipment-manufacturers for a fair amount of basic to intermediate technical analysis. The minimum information required are the mass flow rate, compressor discharge

temperature and pressure at design operating point, number of stages, number of stages with variable guide vanes, casing axial profile, hub axial profile and high pressure spool RPM. This set of information will not generate the original axial compressor design but only an equivalent design that also fulfills commonly used design rules. After obtaining a set of stage temperature, pressure flow speeds and flow angle, approximate 3D blade geometries may be constructed, enabling further numerical analysis. While an ideal numerical simulation encompasses the entire compressor, this is not always feasible. Therefore, the knowledge of these approximate stage flow speeds and flow angles provides a realistic basis for boundary conditions at each stage inlet or outlet without simulating the rest of the compressor.

2. An alternative set of all-positive concentration exponents for fuel and oxidizer, useful at low fuel concentrations, is formulated to complement the original Westbrook and Dryer [17] 2-step reaction mechanism. The sum of the exponents is the same as the original and preserves the use of the original pre-exponent and pressure dependence. The original Westbrook and Dryer [17] 2-step reaction mechanism uses a negative fuel exponent, which causes mathematical difficulties at low fuel concentrations. Between the original and the new concentration terms, the lower of the two is always selected. This new concentration term is able to blend smoothly with the original before low fuel concentrations cause unphysically high reaction rates, which do not correspond with diminishing fuel concentrations. Consequently, the positive concentration

exponents allow generally larger time steps while fuel could be almost fully consumed. However, this has only been tested for mixtures at equivalence ratio 0.7.

1.7 Structure

The present study is organised into the following chapters.

Chapter 2: The Literature chapter begins with providing more background for the research motivation. Some attention is given briefly to the current unfeasibility of large-scale filtering of methane from air. Next, methods related to stage un-stacking axial compressors are examined. Lastly, the chapter closes with a review on hot surface ignition.

Chapter 3: The Methods chapter covers the development of a method that un-stacks an axial compressor. This is followed by the numerical implementation of a 2-step reaction mechanism for methane combustion and the numerical implementation of a hot surface ignition experiment used to validate the selected 2-step reaction mechanism.

Chapter 4: The Results chapter presents the outcomes of un-stacking the LM2500 axial compressor. To assess the validity of the information from the un-stacked LM2500 axial compressor, a set of stage flow angles is used to construct a heavily simplified flow path and the flow

field is assessed via computational fluid dynamics. Concurrently, the 2-step reaction mechanism for methane combustion, embedded in the numerical implementation of the hot surface experiment, is systemically tested at various surface temperatures to identify the temperature that causes ignition. Lastly, the sequence of events occurring on the heated surface is examined in more detail.

Chapter 5: The Discussions chapter presents insights from un-stacking an axial compressor into individual stages, followed by insights from modelling hot surface ignition on heated surface and closes with a qualitative argument for the possibility of hot surface ignition.

Chapter 6: The Conclusions chapter summarises the findings of the present study.

Chapter 7: The Future work chapter identifies lacking aspects of the current set of simulation outcomes and more gas turbine specific information that support building safety cases.

Chapter 2. LITERATURE

The Literature chapter begins with providing more background for the research motivation by covering ignition and leak event in the North Sea, from the process and aerospace industry and an evaluation of selected industry codes and standards so that the plausibility of gas ingested by a gas turbine is substantiated. Some attention is given briefly to the current unfeasibility of large scale filtering of methane from air, which leaves the air intakes of a gas turbine no choice but to allow methane to pass through. Next, methods related to stage un-stacking axial compressors are examined to support building a method that approximates the conditions inside an axial compressor. Lastly, the chapter closes with a review on hot surface ignition to select a suitable chemistry model to simulate towards hot surface ignition at the conditions found in the axial compressor.

2.1 Ignition and leak events

The data reviewed in this section is from the North Sea. In addition, a diesel-engine event and an aero-gas-turbine event, whose report is publicly available, are also reviewed.

2.1.1 Ignition events

Ignition events data comes from the first “Modeling of ignition sources on offshore oil and gas facilities” (MISOF) report [4]. The publically available 2nd MISOF report [5] builds on the first report [4], including a revised leak frequency model. The number of ignited events from United Kingdom Continental Shelf

(UKCS), Norwegian Continental Shelf (NCS) and the Danish Continental Shelf (DCS) is summarised in Figure 2.1. The number of events in each portion of the continental shelf is represented by the large outer most squares and the smaller squares within represent subsets of interest, where the ratio of the area of the squares approximates the proportion of events.

Figure 2.1. UKCS and NCS data from appendix in MISOF [4]

However, these 3 areas are governed differently, giving rise to varying reporting criteria and databases. While the number of ignitions per number of leaks is the ignition rate, this does not indicate the probability of any individual leak event igniting as pointed out in Section 3.7.1 in [18].

Taking a deeper look into the Hydrocarbon Release (HCR) database maintained by the United Kingdom Offshore Operators Association (UKOOA) and the Health and Safety Executive (HSE) for the UK continental shelf, the MISOF report [4] provides a more comprehensive basis for Quantitative Risk Assessments by focusing on major events that typically meet these criteria:

- 1 Defined as "significant" in the HCR database
- 2 Defined as "process leak" in the HCR database
- 3 Flare gas or liquid carry over being ignited by the flare but gas from vents and fuel gas ignited at the gas turbine are not considered relevant
- 4 A leak rate larger than 0.1 kg s^{-1}

The MISOF report [4] identifies 3 major ignited gas leaks events and attributes 1 event fully to ignition by a gas turbine ingesting gas and another event to an equal contribution of ignition by a gas turbine ingesting gas and delayed-ignition. An overview of ignition events related to gas turbines is given in Figure 2.2. One of the major events is attributed to 2 equally likely causes, as elaborated above, giving a “fractional event 0.5”.

Figure 2.2. Ignition events in the North Sea related to gas turbines from data in appendix in MISOF [4]

With half the major events judged to be caused by gas ingestion into gas turbines, the MISOF reports [4], [5] emphasize the need for an improved understanding of the ignition mechanism posed by a gas turbine. While an ignition probability model for the gas turbine is present in Appendix C of [5], the authors of MISOF note that this model remains a hypothesis, which requires further research, numerical simulations and experiments.

2.1.2 Leak events

From events recorded in Reference [18], the top 3 systems (out of 52) reporting the highest system failure rates (most leaks per system-year of operation) were the gas compression system, export oil system and the Utilities, Gas, Fuel Gas system. Incidentally, these systems are also high-pressure systems driven by gas turbines. Guided by the analysis made for Reference [18], the data in the MISOF report [4] from 1992 to 2012 over the UKCS, NCS and DCS showed that a similar group of gas compression, export (condensate, oil and gas) and utilities, oil, gas and power generation turbine systems are related to disproportionately more leaks.

Figure 2.3. Systems related to gas turbines and their contribution to leaks events from data in appendix in MISOF [4]

While these are only leak events, they do indicate that isolating the gas turbine from igniting the leaked gas is equally essential. This concern for explosion safety arising from leaked gas exposed to the external hot surfaces of a gas turbine also motivates the work of Kowalski and Engelmann [19], which is in the context of improving safety levels of smaller distributed power generation facilities consisting of gas turbines producing up to 25 MW.

2.1.3 A leak and ignition event outside the MISOF report

A leak and ignition event is the Deepwater Horizon incident in the Gulf of Mexico, which sadly took the lives of 11 crew members while injuring many others. Investigations for this accident show that ignition of a large gas leak by diesel engine is a likely contributing factor [20], [21] and [22].

2.1.4 Similar incidents in the process industry

A search in a leading journal for knowledge sharing in risk management, reveals records of only cases where causes and solutions are certain. A search for similar documented events reveals that Piper Alpha (1988) is the only offshore fire incident reported. The next most relevant are the few articles on applying reduced order chemistry modelling and ignition probability. Generally, no discussions are found on major fires or explosions on offshore platforms whose accepted cause is the ignition of leaked flammable gas by ingestion into a gas turbine.

2.1.5 A leak and ignition incident in the aerospace industry

A recent engine fire incident (27 June 2016) in the aerospace industry involved a GE90-115B high bypass ratio turbofan engine, which was installed on a Boeing 777-300ER civilian passenger plane. The Transport Safety Investigation Bureau (Singapore) points out the following in their final report [23] for this engine fire.

Fuel is ingested and the engine could maintain normal operation at reduced power setting. Fuel at relatively high pressure leaked into the lubrication oil system and displaced the lubrication oil. The amount of fuel was so high that the fuel overflowed the 2 lubrication oil sumps within the low pressure compressor of the GE90-115B engine, through the variable bleed valve, through the high pressure compressor and onward through the rest of the

engine. When the engine was at high power setting, there were vibrations but no high Turbine Inlet Temperature (TIT) indications to the crew.

Hot surface ignition occurred on the engine when the aircraft slowed down during landing. According to the findings, when the local speed of flow, over the hot parts of the engine that were drenched in fuel, reduced during the actuation of the thrust reverser, hot surface ignition occurred. The thrust reverser actuation is for braking during landing and brings about a rapid speed decrease from moderate to slow.

2.1.6 Summary for ignition and leak events

Both MISOF reports [4], [5] and separate analysis of the same data identified a few major and minor ignited events in the North Sea where the gas turbine is likely the source of ignition. The other events outside the MISOF reports indicate that fuel ingested by an engine is a challenging safety concern.

2.2 Codes and standards for gas turbine operation

There are many codes and standards relevant to gas turbine operation in the oil and gas industry. An example list containing more than 300 codes and standards exists is compiled by Kurz and Brun [24] and a selection is reproduced below.

- ANCI B133.4 Gas turbine Control and Protection System
- API 616 4th edition Gas Turbines for the Petroleum, Chemical, and Gas Industry Services
- API 614 4th edition Combustion Gas Turbine for General Refinery Service
- ISO 2314 1989 Gas turbines - Acceptance tests
- NFPA 12 1989 edition Carbon Dioxide Extinguishing Systems
- NFPA 69 1997 edition Standard on Explosion Prevention Systems
- NFPA 70 2002 edition National Electric Code
- NFPA 70E National Fire Code Errata
- NFPA 72 2002 edition National Fire Alarm Code

- NFPA 85 2001 edition (extract) Boiler and Combustion Systems Hazards Code
- OSHA Noise Procedure Specification
- PTC 1 General Instructions
- PTC 22-1977 Performance Test Code on Gas turbine
- UL 1604 Electrical Apparatus for Explosive Gas Atmosphere

However, the following non-marine and marine codes are selected for discussion as they define the operation gas turbines, air intakes and inert gas systems on marine or offshore platforms.

2.2.1 Non-marine codes and standards

The following codes and standards are discussed in greater detail for their closer relevance to the present study. This discussion is not exhaustive and meant to give only an indication how codes and standards have shaped the way the gas turbine is deployed in the non-marine industry.

The relevant portions of American Petroleum Institute (API) Standard 616 [25] most closely related to removing or reducing ignition probability surrounding the gas turbine are paragraphs 4.1.14, 5.4.1.5 and 5.4.1.5.2. While the gas turbine may be installed in a location identified as generally hazardous, there is no specific mention that the hazard could be ingested flammable gas. The prevention of ingestion of hydrocarbons by filtering is pointed out in paragraphs 5.6.2.3, 5.6.2.3.1 to 5.6.2.3.3. The primary focus of the filtration requirements is removal of large and fine particles. There is no mention of filtering out flammable gas.

According to the recommendations of API Standard 616 [25] for safe gas turbine operation, the vendor is solely responsible for the gas turbine in general while the purchaser is solely responsible for providing an acceptable

environment for gas turbine operations, such as clean air free of volatile organic compounds. The relevant clause for the vendor is 4.1.2. The relevant clauses for the purchaser are paragraphs 5.6.1.9, 5.6.1.9.1, 5.6.1.9.2 and Table 7.

Therefore, the interpretation of API Standard 616 [25] then requires the purchaser to provide air that is free of flammable gas and does not require that air is filtered before entering the gas turbine as a precaution to remove flammable gas. The gas turbine vendor is responsible for safe (hazard mitigated) operation of the gas turbine in general only.

The portions of National Fire Protection Association (NFPA) 37 [26] relevant to gas turbines concern flue gas recirculation and are found in paragraphs 4.1.1.2 and A.4.1.1.2. Flue gas is exhaust gas exiting to the atmosphere via a flue or a pipe. Based on NFPA 37 [26], precautions would be taken to not reintroduce exhaust gas into the gas turbine via the intakes, which might contain trace amounts of unburnt fuel. However, there is no explicit mention of preventing flammable gas from being drawn into the gas turbine. The consideration that air could be contaminated with flammable gas is not addressed.

A related category of equipment that could ingest or accumulate flammable vapours is the Heat Recovery Steam Generator (HRSG), which is governed by NFPA 85 [27]. NFPA 85 considers the risk of gas accumulation through gas dispersion within the HRSG and explosion risk. A purge-credits system is developed to meet the need to balance time spent purging the system against operational flexibility.

The sections most relevant to safety systems handling contaminated air prescribe a minimum purge requirement in paragraphs 8.8.4.2.1.1 and 8.8.4.2.1.2. Depending on the volume enclosed, the purge volume for the combustion turbine can be rather large and takes time to build up. Currently, NFPA 85 provides 3 system designs for maintaining purge credits for the combustion turbine, described in paragraph 8.8.4.6, 8.8.4.6.1 (system 1), 8.8.4.6.2 (system 2) and 8.8.4.6.3 (system 3). Similar to the combustion turbine, the purge volume for the duct burner can be rather large or takes time to build up as prescribed in paragraphs 8.8.5.1 and 8.8.5.2. The current purge credit system NFPA 85 provides to maintain purge credits for the duct burner is detailed in paragraphs 8.8.5.6.1, 8.8.5.6.3 and 8.8.5.6.4.

NFPA 85 notes clearly that explosion risk exists especially when flammable vapours accumulate within the HRSG via the fuel system. Safety has been ensured by positively shutting off the fuel system and providing sufficient air flow rates that remove even stagnant pockets of air. Simulations may provide a cost-effective means for assessing the risk of explosions in operational scenarios and the outcomes may facilitate a review of the tasks performed when purging the combustion turbine and HRSG. Simulations may also provide a means of evaluating alternative engineering controls, which may improve safety.

The European standard EN 13463, specifically 13463-1:2009 [28] and 13463-6:2005 [29] are also relevant for mechanical equipment or engines, in the light

of the present study. Part 1 specifies how to assess the ignition hazard posed by mechanical equipment. According to EN 13463-6:2005 [29], equipment may be constructed with in-built ignition prevention measures, for example sensors and actuators that achieve a minimum quality or minimal performance, graded in “Ignition Prevention Levels”. EN 13463-6:2005 [29] is relevant for gas turbines as they contain potential ignitions sources that can only be prevented from becoming effective ignition sources by measures listed in this standard. The current and only prevention measure unanimously consistent in the industry is however winding down of gas turbine operations when explosive atmospheres are detected.

2.2.2 Marine codes and standards

Marine codes and standards also apply as the platform in the present study is located offshore. Only selected Lloyd’s Register rules are discussed in greater detail. Rulefinder 2014 version 9.21 is used. This discussion is not exhaustive and meant to give only an indication how codes and standards have shaped the way the gas turbine is deployed in the marine industry.

For gas turbines in maritime applications, a gas turbine’s inlet and exhaust ducting arrangements, with its proposed field of application and operational limitations are required by the rules in References [30] and [31]. The focus of this rule is to evaluate the design of intakes to filter out water, particulate and corrosive marine salts. This rule does not explicitly consider the possibility of ingestion of flammable gas through the intake. The next section of the rule focuses on the ability of the gas turbine casing to contain the debris of a blade

release event, and limiting the consequences on other hazardous equipment. In addition, the gas turbine intake should not ingest other harmful objects or ice.

The prevention of unintended accumulation of toxic gases or vapours and their reaction with sea water is addressed in References [32] and [33]. Dust or gas explosion hazards are also noted. These scenarios are mitigated by detecting specific gases, detecting the deficiency of oxygen, and supplying inert gas with inert gas generation systems. However, the considerations about hazardous gases have not been applied to mechanical equipment. This is reasonable since other means and measures separate a large engine, such as a gas turbine from the process plant areas. Gas detection is clearly not new; however, it has been applied to the process plant compartments but not explicitly to the engine compartment.

The rules concerning special service craft driven by gas turbines in References [34] and [35] also focus on gas turbine inlet and exhaust ducting arrangements and filtering out water, particulate and corrosive marine salts.

The rules for natural gas fuelled ships in Reference [36] focuses on explosion risk posed by natural gas and explosion prevention. The use of inert gas is not new. The ventilation air system needs to meet an established minimum specification. Gas turbines may be installed in gas-tight enclosures, which are ventilated to remove heat and other vapours. However, this is not the same as ensuring gas vapours are prevented from entering the air intake. Air intakes are separate ducts from the gas-tight enclosures that house the gas turbines.

Technology to supply inert gas is not new as seen in the familiar requirements for safety zones surrounding charged nitrogen-enriched air and oxygen-enriched air in Reference [37]. While these requirements keep personnel away from oxygen-enriched gases, there is no explicit consideration that inlets are to be protected by active or passive ignition prevention devices or filtration devices.

A similar rule in Reference [38], also emphasizes keeping personnel away from oxygen enrich gases and nitrogen enriched gases. However, there is no explicit consideration that inlets are to be protected by active or passive ignition prevention devices, except to clean and maintain the temperature of the compressed air.

Pressurised inert gas has been used to combat fuel leaks in Reference [39], indicating that purging or dilution by inert gas is not novel. The challenge is to prepare inert gas free of flammable gas, since filtration of flammable gas is not currently feasible.

There are 111 articles related to inert gas in Lloyd's Register rules. Generally, inert gas has been used to ensure safe handling of flammable cargo and fuel. The possibility of engine or gas turbine intake air being contaminated with flammable gas is nevertheless not mentioned.

Concerning gas turbines for ships in Reference [31] and naval ships in Reference [40], the filtration of water, particulate and corrosive marine salts at the air intake is emphasized, as this is an equipment manufacturer's requirement. Filtration of flammable gas is not mentioned.

A gas turbine shut down is triggered mainly by over temperature as most forms of degradation cause a temperature rise while compensating for reduced performance. The rules call for safe gas turbine wind down according to Reference [41] and Reference [42] by shutting off the fuel supply to stop the gas turbine.

2.2.3 Statutory rules of the International Maritime Organisation

Inert gas on a marine vessel traditionally comes from an oil-fired gas generator using flue gas and is used primarily to keep the space of the cargo hold non-flammable or below its LFL [43] and [44]. There is no mention of engines operating in runaway mode (rightly so as there are numerous regulations concerning avoiding off-design scenarios) and no mention of using inert gas to stop runaway engines. To supply inert gas to an engine intake, oil-fired flue gas is a reasonable source of inert gas. In section 4 of [44], engines are not considered a source of ignition in the marine context.

2.2.4 Equipment operating in explosive atmospheres

The standard EN 50303 [45] is primarily for the equipment that must operate in explosive atmospheres in the mining industry as seen in Section 3.6 Paragraph

2 and Section 4.1.1. However, EN 50303 has not been applied to the gas turbine.

2.2.5 Summary for codes and standards for gas turbines

To the best knowledge of the author, the selection of codes and standards discussed briefly in the preceding sections are the most relevant for gas turbines, air intakes and inert gas systems. These paint an approximate picture of the industry's view of the relationships between ignition risk, flammable gas and gas turbines. From these, it is clear that a scenario that air could be contaminated with flammable gas is seldom addressed and this leads to no mention of requirement to filter out flammable gas. The scenario of flammable gas entering the gas turbine air intakes is not discussed. However, the filtration of water droplets, particulates and corrosive marine salts is a major purpose of gas turbine air intakes.

The codes and standard however do acknowledge that explosion risk exists especially when flammable vapours accumulate and that inert gas generating system are a reliable way to reduce flammable vapour concentrations below LFL. Till date, the gas turbine does not encounter any standard that requires it to operate within explosive atmospheres hence the ignition risk posed by a gas turbine when inadvertently operating in an explosive atmosphere is largely unknown.

2.3 Detecting and separating methane gas from air

The turbine package is an enclosure that contains the gas turbine with all associated equipment. The minimum features are the intake ducts, exhaust stacks and driven equipment or output drive shaft. The most relevant feature to the present study is the mechanical filters that remove particulate contamination in air, including heavier, more viscous hydrocarbons.

2.3.1 Detecting methane in a gas turbine

In the present study, apart from the major assumption is that the gas detector system will detect a gas leak, the gas turbine will show signs of burning excess fuel. To the gas turbine, this ingested methane gas from an external leak will be additional fuel, which certainly increases a gas turbine's turbine inlet temperature and high-pressure spool (compressor and turbine) rotational speed, among other consequences.

2.3.2 Separation of methane by molecular sieving

A very cost effective means to reduce erosion on the gas turbine compressor blades is using high efficiency particulate air filters to remove particulates. As these filters cannot filter out methane to butane gas; the feasibility of filtering methane is explored next.

The possibility of separating methane from air does exist. Shakocius and Miller [46] demonstrate the feasibility to concentrate oxygen from air using pressure swing adsorption and a single adsorbent zeolite molecular sieve to obtain 95% pure oxygen. This 95% pure oxygen is then passed through a carbon molecular

sieve to remove the remaining Argon gas to obtain more than 99% pure oxygen. The mole fraction of contaminant methane is 0.005 and is fully removed at the end of the zeolite molecular sieve. The zeolite molecular sieve is a synthetic, alkali-metal, alumino-silicate material with uniform pore sizes of 7.4 Å within a 13X type crystal structure. The pore sizes in the carbon molecular sieve are not uniform but narrowly distributed. This is a laboratory scale demonstration where the inlet pressure is about 3 atm and the production rate is 0.001 m³ oxygen purer than 99% at standard temperature and pressure per minute. The inlet pressure requirement could be reduced since only methane needs to be removed and not all nitrogen, yielding a modified product at a higher rate.

The review by Smith and Trimm [47] points out the poor availability of commercial membranes for gas separation. The most promising methane separation membranes still under development are silica, DDR zeolite membrane and Sr-ETS-4 zeolite membrane. DDR refers to “Deca-dodecasil 3R” and is a type of pure silica SiO_2 zeolite, whose pore system is constructed out of 19-hedral cages interconnected through 8-ring windows with an aperture of about 3.6 by 4.4 Å [48]. Sr-ETS-4 refers to a family of stable, small-pore crystalline titanium silicate molecular sieve zeolites consisting of Sr^{2+} cations, TiO_2 , SiO_2 and water [49]. However, membranes tend to be costlier compared to the pressure swing adsorption and temperature swing adsorption approaches.

Instead of filtering out methane, coal mines operators have turned to using methane in ventilation air as an energy source. Baris [50] gives an overview of applicable technology and the preliminary analysis of the economic feasibility of

harnessing methane in ventilation air at the Kozlu mine in Turkey. The overview also points out a lean-burn gas turbine technology, which uses methane at low concentrations of 0.8 % to 1.6 %.

2.3.3 Enhancing gas separation through pressure changes

The vacuum pressure swing adsorption method, with a modified carbon molecular sieve is investigated experimentally and theoretically by Yang et al. [51], to separate methane from methane and nitrogen mixtures. The raw mixtures consist of methane at 10%, 30% and 50% by volume, where the smaller amount of methane approximates a coalmine methane mixture. Their process uses high pressure at 500000 Pa and a low-pressure vacuum at 20000 Pa. The temperature is constant at 293 K. The vacuum step enables the process to yield higher purity methane, against the major species nitrogen.

2.3.4 Preferential molecular sieving

Alternatively, instead of alternating adsorption and release from a molecular sieve, Shang et al. [52] synthesised a class of chabazite zeolites to “molecularly sieve” based on the ability of a guest molecule to induce temporary and reversible cation deviation from the center of pore apertures in the zeolite. This allows for exclusive admission of certain molecules, which permits separation by “size-inverse” discrimination. Through experimental and computational approaches, the underlying mechanism was found similar to a “molecular trapdoor”. With their materials, they demonstrated the case of admission of a larger molecule CO_2 in preference to a smaller molecule CH_4 , achieving the highest selectivity of CO_2 over CH_4 . They found that carbon dioxide slips past

the cation due to its electron-rich oxygen atoms. The targeted applications are removing inert gases in natural gas streams and purification in carbon capture schemes.

2.3.5 On-board oxygen generating system

Commercial maturity of molecular sieving is demonstrated in on-board oxygen generating system (OBOGS). This oxygen-on-demand system demonstrates the reliability of molecular sieving to deliver stable low flow rates. This worked example estimates the mass flow rate of clean air.

$$\begin{aligned} &0.000125 \text{ m}^3 \text{ s}^{-1} \text{ (7-8 liters of air per minute per person) } \times \\ &1.204 \text{ kg m}^{-3} \text{ air density (Normal temperature and pressure, an} \\ &\text{approximation of cabin conditions) } \times \\ &450 \text{ passengers (the B777 is able to sit 451 passengers) } \\ &= 0.067725 \text{ kg s}^{-1} \\ &[\text{https://health.howstuffworks.com/humanbody/} \\ &\text{systems/respiratory/question98.htm assessed 09 June 2015}] \end{aligned}$$

The flow rates required by the gas turbine in the present study is about 68.2 kg s⁻¹ at the maximum power setting, which far exceeds the OBOGS delivery by 1000 times. Molecular filtration of methane is possible; however, it is unlikely to provide viable flow rates for gas turbines.

2.3.6 Respirator for personal safety equipment

A survey of respirator products for personal safety shows that methane gas is not filtered and to prevent inhalation, a self-contained breathing apparatus is required. On offshore platforms, the two gases which pose the greatest safety concerns are corrosive hydrogen sulfide and flammable methane. Till date, methane is prevented from entering a diesel engine by closing a “Rigsaver” type valve, either automatically or manually.

2.3.7 Summary for filtering methane

There are no membranes or filters that may rapidly and efficiently separate methane from large volumes of air. Without a suitable membrane or filter integrated into the air intakes of a gas turbine package, methane gas is still able to pass through the filters and into the gas turbine.

2.4 Stage stacking of axial compressors

Despite its relative simplicity, the 1D analysis at the mean line has a great fundamental influence on the design of an axial compressor as this is where each stage's pressure and temperature ratios are defined before any stage is designed in detail and the stages assembled together. In 1D analysis through the turbomachine, the corrected mass flow rate is examined for the effects of pressure. Because the mass flow rate, effective flow area and pressure are in an intricate relationship, Cumpsty [53] highlights that obtaining correct stage stacking or matching will be challenging. The gas turbine developed along traditionally distinct components lines and each major component has been refined tremendously to achieve efficiencies over 90%. The design space is now arguably more complex owing to more disciplines, including interdisciplinary work. Ghisu et al. [54], [55] have developed an integrated design approach using a 1D mean line solver embedded in an optimisation routine. Their approach defers fixing the components interface design parameters till later phases in the design process, resulting in better explorations of the design space and hence harnessing the gains from trade-offs between different components and disciplines. From the observations of Jarrett and Ghisu [56],

the search for an optimised balance between time spent on configuration selection and refining a selected configuration during the design process reveals that in the best designs, configuration selection with 1D mean line solvers consumes half to three-quarters of the design time.

The stage stacking process is at the core of 1D analysis at the mean line. The stage stacking approaches in the literature focus on building up a compressor stage by stage, using known stage inlet flow angles, stage temperature ratios and pressure ratios or equivalent information. For the gas turbine manufacturers, the design process for each stage may be guided by design values and rules developed in previous compressor designs. Sehra et al. [57] apply existing knowledge and design techniques from an aviation gas turbine to design the compressor of a utility gas turbine. Smed et al. [58] report evolving the design of compressor within a family of gas turbine models. Smith [59] began unifying compressor models into families based on similar design rules. Mattingly [60] shows that the design process is often iterative as a multitude of performance requirements must be fulfilled simultaneously. Apart from configuration selection, another main purpose of 1D stage stacking methods is to provide an efficient alternative for estimating a compressor's performance map, including an estimated safety margin the operating line has from the stall line and from the choke line. The non-manufacturers may use stage stacking to infer the main features of an actual compressor's design and compare the obtained compressor performance map against known data from manufacturers in an iterative process as performed by Seddigh and Saravanamuttoo [61], and also by Lakshminarasimha et al. [62] for the purposes of their own work. In the light

of this, the stage flow angles, flow speeds, stage characteristics, among other variables are then the inputs to the stage stacking method. The ability of the blades profile to maintain attached flow at reduced or excessive mass flow rate within a range of off-design flow angles are derived from experimental data or from performance data of a previous related design.

When faced with a task to determine the stage details of a multi-stage axial compressor designed by others, the current methods require a large number of inputs, which may not be estimated with certainty. While estimates and design guides may be helpful sources of input for design variables, there are few systematic ways to un-stack a multi-stage axial compressor, other than iteratively testing with a range of input values for each design variable. The available information on an axial compressor is usually the overall pressure ratios and the overall efficiency, hardly mentioning how flow angles and flow speeds relate within the machine. The aim of the present study is thus to present a stage un-stacking method that uses minimum information and applies a feasible relationship between adjacent stage temperature ratios and stage pressure ratios, to infer the stage flow angles and stage flow speeds for the axial compressor operating at the design point. Presently, this method is applied only at a compressor's design operating point. While 2D streamlines curvature methods are the common approach to define the blade geometry and flow angles at each axial stage in relation to the next axial stage, the present study details a 1D approach that trades off realistic flow physics at blade surfaces for quicker calculation of the mean flow variables.

2.4.1 RSRR approach

The Repeating-Stage Repeating-Row (RSRR) model from Mattingly [60] is discussed first as it is also introduced in an aircraft engine design book by Mattingly et al. [63]. This design approach is the simplest and therefore provides a suitable initial design. Each stage has the same axial velocity, constant mean line radius, inlet angles and outlet angles. Consequently, the stage degree of reaction is fixed at 0.5.

2.4.2 STGSTK code

The STGSTK code by Steinke [64] is an early code used to predict the off-design performance of an axial compressor based on operation at design conditions. The STGSTK code is also referred to as “A Computer Code for Predicting Multistage Axial Flow Compressor Performance by a Meanline Stage Stacking Method”. The analysis is performed at the mean-line with velocity triangles at the rotor inlets and outlets. The compressor is built up cumulatively through stage stacking to obtain the multistage design and overall performance. The input parameters required to describe the design condition are the Stage Flow Coefficient (SFC), the stage total pressure ratio, and the stage adiabatic efficiency. The stage adiabatic efficiency as a function of SFC summarizes the aerodynamic performance from choke to stall for the airfoils in the blade row. This efficient approximation uses two parabolic curves to describe the variation of efficiency from choke to stall. To model off-design operation, the mass flow rate at choke and mass flow rate at stall, and part speed are required to determine the expanded range of SFC. The code then modifies the stage total pressure ratio and the stage adiabatic efficiency characteristic curves to

produce related off-design stage characteristic curves. This code has been tested by Steinke to predict a compressor performance and a single stage performance with Inlet Guide Vane (IGV) resets, generating predicted stage characteristic curves which are close to measurements for stage total pressure ratio and the stage adiabatic efficiency. However, the few critical parameters that build the compressor stage by stage are required inputs to STGSTK instead of outputs; therefore, the STGSTK code is unable to provide guidance on the stage-to-stage variation of these critical parameters.

2.4.3 LUAX-C code

A recent 1D steady state operation stage stacking model is the Lund University Axial flow compressor (LUAX-C) in Falck [65]. This model is under active development again in 2013 by Perrotti [66]. This model is much more flexible than the RSRR model and has the potential to obtain most of the geometric, thermodynamic and flow conditions in each blade row of each stage. A number of experimentally based enhancements were incorporated, such as empirical relations for incidence angles and deviation angles at each blade row, blade profile losses and endwall losses. However, this model was not used as it required stage solidity and stage reaction as inputs. Another required input was stage load distribution which had to be arbitrarily specified from compressor inlet to outlet. Compared to the RSRR approach and the STGSTK code, more inputs are required in LUAX-C, as fewer assumptions are made.

2.4.4 Stage pressure ratio distribution

In Figure 2.4, the pressure ratio distribution of the LM2500 compressor is compared to another compressor by the same manufacturer, “PR GE NASA EEE” referred to by Bruna et al. [67] and a similar 17 stage machine by Kashiwabara et al. [68], “PR Hitachi 17 stg”. On the horizontal axis for normalised stage number, the inlet is at 0 and the outlet is at 1.

Figure 2.4. Pressure ratio distribution vs. normalised stage number for selected axial compressors

The LM2500 and Hitachi 17-stage are land based turbines. In the design of the Hitachi 17-stage compressor, the front 3 stages are highly loaded [68]. The LM2500 compressor does not deliberately load the front stages. While the design perspectives differ, the stage pressure ratio distributions are similar with a peak in pressure ratio at one of the front stages. The “GE NASA EEE” refers to the Energy Efficient Engine (EEE), meant to support aviation engine development. The detailed design phase for the “GE NASA EEE” compressor began with specifying the specific stagnation temperature rise at each stage for the design operating point, as seen in Holloway et al. [69]. This distribution was overall decreasing with stage number except the middle stages 6 and 7, where the decrease was more obvious. The initial distribution of the stage static temperature rise in Holloway et al. [69] is similar. In the final configuration, the

static temperature distribution through the stages did not change too much as seen also in Holloway et al. [69]. While the pressure ratio was not specified directly, the obtained pressure ratio in Bruna et al. [67] synchronizes closely with the temperature variation in Holloway et al. [69].

A gas turbine may also see different design approaches in its development journey. Smith [59] documents the rich design heritage of the LM2500 gas turbine which has experienced 2 rounds of stage additions at the rear. While there is little doubt of an improved understanding of the underlying physics of flow and of materials, the account by Smith [59], shows instead that the proven aspects of the current design are retained in the interest of reliability when adding more stages. Wadia et al. [70] report the most recent addition of the 0th stage to the front of the compressor where little of the original gas turbine is altered.

2.4.5 Deliberately working with limited data

Stage stacking methods demand increasing inputs to generate more feasible designs capable of more realistic performance prediction. This is not a challenge for the knowledgeable original equipment designer. However, the reminder of the non-designers looking to analyse the axial compressors and have no intimate access to one, the available information tends to be sparse. A few pieces of certain information for the studied axial compressor are taken from Pedersen [15] and they are:

- h , vane height (m)
- s , vane density (m)
- c , chord (m)
- RMS , mean line radius (m)

- A , flow area (m^2)
- P_{OUT} , load on power (kW)
- P_2 , static pressure at the compressor outlet (Pa)
- T_{TOT3} , stagnation temperature at the compressor outlet (K)
- $\dot{m}_{\text{AIR}}$, mass flow rate (kg/s)
- ω , shaft rotational speed (RPM)

Due to a lack of precision in the data, the number of blades could not be determined from the mean line radius and vane density values. Subsequently, while blade solidity may be obtained from the chord to vane density ratios, the use of solidity values is avoided. The chord information is not used as it alone was not sufficient to fix the axial locations of each stage with certainty. Without more information for analysis, the conditions at the compressor inlet are assumed to be 278.15 K and 100000.0 Pa. The overall static pressure rise, for the studied axial compressor from Pedersen [15], is estimated at 1.719×10^6 Pa. A few data points seem erroneous and were replaced by interpolated values. Since the set of operation data from Pedersen [15] and Pedersen [6] for the compressor inlet and outlet is used as the main input, this has heavily influenced the hard coding of the stage un-stacking method.

2.4.6 Information sources

To supplement the insufficient information gathered in the previous section, the sources of inputs for stage un-stacking an axial compressor is restricted to publicly available and conveniently accessible information. No further inputs are sought from either the original equipment manufacturer or equipment owners, so that the proposed method is also applicable for preliminary analysis of other designs and by students without access to extensive libraries of gas turbine information. For the model of axial compressor examined here, there is much more information available from Klapproth et al. [71] and Wadia et al. [70]. To

develop a robust method capable of estimating a compressor's mean line performance close to the actual, information in Klapproth et al. [71] and Wadia et al. [70] are not used to develop the stage un-stacking method but only in validating its effectiveness. The information from Pedersen's [15] is the only information used to begin the present study.

2.4.7 Summary for stage stacking of axial compressors

Axial compressor design approaches inevitably require much information even for a basic design. The contention is summarised in Table 2.1 Table 2.2.

Table 2.1. Contrasting characteristics of the stage stacking and stage un-stacking processes

Stage stacking	Stage un-stacking
1. Original Equipment manufacturers	1. Owner, operators, 3 rd party independents
2. Engineers designing from scratch	2. Engineers but non-designers
3. Design trade-offs are known	3. Unable to infer the design trade-offs
4. All data is potentially available	4. Available data is sparse
5. Analysis outcomes are mostly confidential	5. Confidential reasons for further analysis
6. Only essential details shared publically	6. Unable to share problem statement

2.5 Hot surface ignition and auto ignition

The majority of the literature focuses on the time delay of auto ignition of quiescent premixed flammable gas and air at a temperature exceeding the auto ignition temperature. This has culminated in the accepted ASTM E659 test method [72], which is adopted as the method to determine the Auto Ignition Temperature (AIT) in API Recommended Practice 2216 3rd Ed. (API RP 2216) [73]. This recommended practice states that in common situations, the contact time of flammable gas on hot surfaces is very limited, especially when in the open with convection and winds to consider. Therefore it is concluded that surfaces must be at least 182 K above the AIT for auto ignition to occur in these situations [73]. This however, does not apply to the situation in the present study. The closest data for flowing flammable gas and air mixtures over a

heated surface is available from only one source: Smyth and Bryner [1]'s experiment, but for a small surface.

2.5.1 Auto-ignition simulations and experiments

According to API RP 2216 [73], the definition of Auto-ignition Temperature (AIT) is “the minimum temperature required to initiate or cause self-sustained combustion independent of an external ignition source”, which is similar to that in Babrauskas [74]. The data source for AIT is then the minimum temperature at which auto-ignition occurs under the specified conditions of the ASTM E 659 test. The ASTM 659 test puts a *stagnant* mixture of flammable gas and air in contact with the heated internal surface of a borosilicate round bottom flask [72]. Robinson and Smith [16] did similar work using an approximately spherical stainless steel test vessel but put their methane-air mixtures in contact with both stainless steel and with a layer of oxide simulating a glass surface. They reported a 7 K to 12 K higher ignition temperature when the gas mixtures are in contact with the stainless steel surfaces (Figure 1.2).

However, ignition temperatures obtained from enclosed small volumes of flammable gas mixtures are not representative of gas mixing in an open-air environment. It is deemed highly improbable for hot surfaces to ignite hydrocarbon vapours at the lowest published AITs, considering convection and winds dispersing the flammable gas. API RP 2216 [73] concludes that should ignition take place, this happens only for surface temperatures that are 182 K above the minimum ignition temperature for the flammable gas, limited mostly by short contact durations with the heated surface. API RP 2216 [73] also points

out industry experience where flammable gas leaks near surfaces which are a few hundred degrees hotter than minimum ignition temperature but do not ignite. However, API RP 2216's [73] conclusion is for an open air environment, and therefore not automatically valid for internal flow over the heated internal surface inside a gas turbine engine, where the mixture is not dispersed and the contact duration with the hot surfaces can be long.

The collection of laboratory based open air tests referred to by API RP 2216 [73] is carried out by Smyth and Bryner [1]. The study of Smyth and Bryner [1] focuses on scenarios where the flammable gas experiences a short-duration exposure to the hot surface as this is relevant for dangers arising from equipment malfunctions and leaked gas. In their experiments, a flammable gas mixture jet impinges a small heated surface at an angle. Ignition is detected by the visual onset of flames and through thermocouple readings.

The process parameters considered most important are:

- surface temperature
- surface size
- surface orientation (relative to flow)
- initial mixture temperature
- residence time (alternatively, speed of flow over the surface, which unfortunately also effects the heat transfer coefficient)
- condition of surface (smooth to rough)

The major differences between methods according to ATSM E659 [72] and to Smyth and Bryner [1] are summarised in Table 2.2.

Table 2.2. Contrasting the ASTM E659 method and Smyth and Bryner [1]'s experiment

ASTM E659	Smyth and Bryner
<ul style="list-style-type: none"> • 10 min duration • Gas sample injected into a round bottom flask containing air • Curved surface of flask • Glass surface • Flask internal surface area • Surface heated indirectly • Closed system • A single injection of gas • Flow is stagnant and volume is fixed 	<ul style="list-style-type: none"> • Short duration of less than 150 ms • Gas-air mixture effectively premixed • Flat surface at 45° angle • Metallic surface • Small surface area compared to flask • Surface heated directly • Open loop flow • Continuous supply of gas • Mixture mass flow is controlled at a volume flow rate of $1.52 \times 10^{-5} \text{ m}^3 \text{ s}^{-1}$ and speed of 0.16 m s^{-1}

To the author's knowledge, Smyth and Bryner [1]'s experimental work is the only study with flowing flammable gas over a heated surface and comprehensively documented. This is still a flow test over a small surface in open air, so the results cannot be immediately applied to an internal flammable gas flow fully enclosed and heated by the internal surfaces of a gas turbine engine. However, by lack of more suitable data, this experiment is used to qualitatively validate the proposed chemistry model in the present study.

The literature reveals further industrial experimental research; however, the studies are using simple geometries enclosing a stagnant flammable mixture and do not consider the effect of flowing flammable gas and air mixture over a heated surface. Üngüt and James [75] experimentally determined the AIT of methane, natural gas, propane and butane mixtures with air in a box with cling film walls. The mixture within the box is sufficiently stirred till almost homogeneous and it effectively stationary before the experiment begins. The heating element is positioned facing downward and flush with a ceramic board suspended within the box. The results indicate an increasing AIT with increasing equivalence ratios. Üngüt [76] carried out 3D simulations for alkane

auto-ignition by a heated metal surface, taking into account detailed reaction chemistry and the effects of buoyancy. However, since the flammable gas and air mixture is effectively quiescent, the results are, to the case presented in the present study, useful only to qualitatively verify the obtained trends in AIT of a flowing mixture across varying equivalence ratios. Bjarne, Rasmussen and Sødning [77] propose an ignition parameter definition and carried out experiments with a flammable gas and air mixture flowing in a tube and passing around a heated pellet. Unfortunately, the experimental setup is insufficiently described and therefore a simulation case could not be defined for model validation purposes.

Recently experimental research is carried out by Menon et al. [78] to gain insight into the hot surface ignition process for practically relevant fuels such as heavy hydrocarbon fuels typically used in aircraft engines. The aviation fuels are represented by n-hexane and n-heptane and mixed with air. The mixture is heated by a glow plug in a closed fixed volume pressurised vessel. Thermocouples, pressure transducers and Schlieren imaging are used to detect ignition. A corresponding simulation with detailed reaction mechanism for n-heptane is carried out to gain insight into the transient hot-surface induced ignition process.

A very concise summary of how Computational Fluid Dynamics (CFD) software for fire and explosions implement their ignition models is given by Pedersen et al. [79]. They point out KFX-EXSIM employs the Eddy Dissipation Concept and that FLACS employs the Burning Velocity Model. The Eddy Dissipation Concept

assumes fast chemical reaction rates which always progress the reactions to chemical equilibrium. The Burning Velocity Model relates the chemical reaction rates to the turbulent flame speed and velocity of fresh reactants entering the reaction zone. The reactants also mix infinitely fast.

The ignition criterion developed by Pedersen et al. [79] through a numerical study has 3 parts. First, the mixture must be within flammability limits. Second, the heat lost from the fluid to the wall must equal the heat generated by the chemical reaction. Third, ignition delay must be met. This ignition criterion is applied on a reaction that progresses according to a reaction progress variable whose source term is obtained from the BVM model implemented in the CFX CFD software.

2.5.2 Reaction mechanisms for hot surface ignition

A number of reaction mechanisms are possible. The simplest is a 2-step reaction mechanism reported by Westbrook and Dryer [17], used for its capability to output suitable adiabatic flame temperatures for the range of temperatures and equivalence ratios of interest in the present study. Based on the sequential burning of typical hydrocarbons, this 2-step mechanism is constructed from the Dryer and Glassman modification of the 1-step reaction for the oxidation of methane in a reactor with turbulent flow. In step 1, methane and oxygen react to form carbon monoxide and water. In step 2, carbon monoxide and oxygen react in a reversible reaction to produce carbon dioxide.

The presence of more reversible reaction reduces the tendency of temperature overshoot. The slightly more complicated mechanism by Seshadri and Peters [80] has 4 steps and consist of reversible reactions for carbon monoxide-carbon dioxide and oxygen-hydrogen and 1 radical recombination reaction. Carbon monoxide is produced with hydrogen in step 1 before turning into carbon dioxide and water in the reversible reactions. This mechanism would be suitable for reactions at the surface. Another 4-step reaction mechanism is from Jones and Lindstedt [81], with similar characteristics but no reaction with radicals. This removes the possibility of reactions on the surface.

An example of another more detailed reduced reaction mechanism is Sung, Law and Chens' [82] 15-step reduced mechanism which simplifies the effects of oxides of nitrogen on the reaction. An ideal detailed reaction mechanism is the GRI-Mech 3.0 [83], which incorporates the full effect of all species. As the purpose of the reaction mechanism is primarily correct temperature during ignition, a few reversible reactions suffice instead of a much more comprehensive mechanism. However, when combining a gas-phase reaction mechanism with surface reactions to match a material's ignition temperature, a larger variety of radicals support more individualised tuning of the surface reactions. The effect of radical reactions on a surface is modelled by Sano and Yamshita [84], by simulating 2 theoretical surface conditions: deactivating all radical species upon contact with the surface and using an inert surface. While using 18 chemical species and 61 elementary reactions, their simulation outcomes indicate that as more radical species are deactivated on the surface, the ignition delay increases. The largest delay comes about when the methyl

radical is deactivated. The radical species are deactivated by specifying their mass fractions as zero on the surface and not with a set of elementary reactions tailored to the surface material.

2.5.3 The Van't Hoff ignition criterion

A precise definition of the onset of ignition by a heated surface is formulated in the Van't Hoff ignition criterion as referred to and applied in the steady state analysis of thermal runaway by Laurendeau [85]. The onset of ignition by a heated wall, as defined by the Van't Hoff ignition criterion, occurs when the temperature gradient at the wall becomes zero. In such case, at that location the rate of heat transfer from the wall into the gas equals the local rate of heat generated by the chemical reaction. The Van't Hoff ignition criterion states that the temperature gradient perpendicular to the wall surface is zero at the onset of ignition, such that

$$(dT/dn)_{\text{WALL}} = 0 \quad (2.1)$$

Laurendeau [85] used Equation (2.1), where n is the direction perpendicular to the wall. The Van't Hoff ignition criterion cannot be used for cases with constant heat flux on the wall and when temperatures approach the adiabatic flame temperature inside the domain. Both are not relevant here.

2.5.4 Summary of hot surface ignition chemistry

In short, Smyth and Bryner [1] is the only available experimental study that has flowing flammable gas and air mixture over a heated metal surface. The effect of surface material is considered by Smyth and Bryner as well, but is not taken into account in the numerical study presented here, as the model is limited to

the ignition phenomena by gas phase chemistry: not taking into account catalytic or radical quenching chemistry on the hot surface.

Chapter 3. METHODS

The Methods chapter covers the development of a method that un-stacks an axial compressor to determine the stage temperature, pressure, flow speeds and flow angles within a multistage axial compressor. This is followed by the numerical implementation of a 2-step reaction mechanism for methane combustion and the numerical implementation of a hot surface ignition experiment used to validate the selected 2-step reaction mechanism.

3.1 Assumptions and supporting information

An illustration of the gas turbine is the present study is shown in Figure 3.1.

Figure 3.1. The GE LM 2500 gas turbine and major components

The gas turbine station numbering from Pedersen [6] is reproduced in Figure 3.2.

Figure 3.2. Gas turbine station number used in Pedersen [6]

The following assumptions and supporting information in Table 3.1 assist the present study by providing realistic estimates for lacking information.

Figure 3.3. Quadratic equations fitted to the compressor casing and hub walls

Table 3.1. Assumptions and supporting information in the present study

Assumption or Information	Supporting information
1. Inlet temperature – 278.15 K. Assume the LM 2500 gas turbine data Pedersen [15] uses is from operating in the higher latitudes of Norway since no further data available.	<ul style="list-style-type: none"> • Lower limit – 274.15 K, World Sea Temperatures for North Sea [86]. • Mean – measured ambient 282.95 K and 97090 Pa at Sleipner gas field (250 km west of Stavanger, Norway), Flesland [87]. • Upper limit – 288.15 K, based on inland test facility and adjusted to ISO conditions, BS ISO 3977-2:1997 [88]. • Note – In Section 2.2.1 of [6], Pedersen uses an air density of 1.2 kg m^{-3}. Therefore, the inlet temperature would be 293.15 K, according to [89]. The density value Pedersen uses does not seem to consider the local temperatures on North Sea.
2. Pressure drop across inlet filter of turbine package – 1325.0 Pa.	<ul style="list-style-type: none"> • Varies widely depending on the maintenance perspective of the operator of the gas turbine. The sea level ambient air pressure is set at 101325 Pa [90].
3. Pressure at outlet of the turbine package – 1325.0 Pa above sea level ambient air pressure.	<ul style="list-style-type: none"> • Arbitrarily approximated such that exhaust will exit the turbine package.
4. Ideal gas model used.	<ul style="list-style-type: none"> • Other more comprehensive gas laws such as Redlich-Kwong (1949) or Guggenheim (1965) give < 1% difference for the pressures encountered.
5. No losses in the slightly divergent duct between the turbine outlet and power turbine inlet.	<ul style="list-style-type: none"> • All stagnation quantities conserved.
6. Polytrophic efficiency > 90%.	<ul style="list-style-type: none"> • A set of polytrophic efficiency estimates for each gas turbine component is given in Table 4.4 of [91]. The LM2500 gas turbine first operated in 1960s and at 2015, its compressor sits in technology level 4 with polytrophic efficiency of 90%. • As these polytrophic efficiencies are for aircraft engine components, it is reasonable that the LM2500 gas turbine, since developed from an aero-derivative base could attain component polytrophic efficiency above 90% after optimisation for sea level power generation.
7. Estimation of hub and casing radius and axial coordinates of each stage from a compressor schematic on the gas turbine manufacturer's marketing datasheet [92].	<ul style="list-style-type: none"> • A quadratic polynomial is the lowest order necessary to return a smooth variation of the casing, mean and hub radius (Figure 3.3). However, a minimum third order polynomial is recommended for future work as this considers that the Navier-Stokes equations contain second order spatial derivatives of velocity.

3.1.1 Heat rate and heating value of fuel

The lower heating value LHV of fuel spans a large range, especially for gas turbines running on natural gas. A specific LHV fixed for the present study is obtained through the heat rate found in [93] and the highest power output P_{OUT} in [15].

$$HR = \frac{\dot{m}_{FUEL} \times LHV}{P_{OUT}} \quad (3.1)$$

However, the heating value is not exact as the power output might receive small contributions from entrained fuel in the intake air. The enthalpy addition during combustion is inferred from the overall efficiency η and power turbine output.

$$\eta = \frac{h_8 - h_{48}}{h_{23}} \quad (3.2)$$

Considering the enthalpy addition from fuel, the enthalpy h_3 at the combustor outlet gives a temperature slightly lower than the given T_3 .

$$h_2 + h_{23} < h_3(T_3) \quad (3.3)$$

3.1.2 Entrained fuel in air

The small difference causing the inequality in Equation (3.3) allows the reasonable assumption that there is entrained fuel in the intake air. Additional enthalpy h_{23EXT} is attributed to entrained fuel to make up the small temperature difference.

$$h_2 + h_{23} + h_{23.EXT} = h_3(T_3) \quad (3.4)$$

It is unlikely that entrained fuel is measured. Therefore, the measured power output consists of a small contribution from entrained fuel alongside the main contribution from the fuel system. Using the overall efficiency on power output,

$$P_{\text{IN}} = \frac{P_{\text{OUT}}}{\eta} \quad (3.5)$$

and applying a small coefficient $k_{\text{POW.EXT}}$ to partition the power input,

$$P_{\text{IN.EXT}} = k_{\text{POW.EXT}} P_{\text{IN}} = k_{\text{POW.EXT}} \frac{P_{\text{OUT}}}{\eta} = h_{23.\text{EXT}} \frac{1}{3} \dot{m}_{\text{AIR}} \quad (3.6)$$

the coefficient $k_{\text{POW.EXT}}$ sets $h_{23.\text{EXT}}$, that brings h_3 and T_3 to the required levels, is found. The air-fuel ratio (by mass) from Pedersen [15] is 48.61:1, using intake air mass flow rate 68.20 kg s^{-1} and fuel mass flow rate 1.403 kg s^{-1} . If fuel contains only methane and air, and air comprises nitrogen and oxygen in a molar ratio of 3.75:1 with 1% Ar (by mole fraction), then the stoichiometric air-fuel ratio (by mass) is 17.32:1. This puts the intake air at approximately 2.8 times the stoichiometric requirement. The argument that about a third of the intake air gives up its entrained fuel to contribute the additional enthalpy input $h_{23.\text{EXT}}$ is reasonable. This helps estimate the amount of entrained fuel in air at less than 1 % by mass or mole fraction.

At the power turbine outlet, it is found that

$$P_{\text{OUT}} > (\dot{m}_{\text{AIR}} + \dot{m}_{\text{FUEL}}) W_{\text{OUT48}} \quad (3.7)$$

which implies that work output W_{OUT48} is lower than required. There is room for entrained fuel to combust, giving an additional work output $W_{\text{OUT48.EXT}}$ to make up the difference.

$$P_{\text{OUT}} = (\dot{m}_{\text{AIR}} + \dot{m}_{\text{FUEL}}) (W_{\text{OUT48}} + W_{\text{OUT48.EXT}}) \quad (3.8)$$

This additional work output must remain below the total possible work output.

3.2 Design rules for an axial compressor at the design operating point

Stage stacking assembles individual stages at the design operating point, where the incidence angle at the blade leading edge is small, the flow of the working fluid follows the curvature of the blade and the velocity triangles at the stage outlets are very similar to the velocity triangles at the following inlets. To un-stack an axial compressor, the following arguments are presented in support of the suggested design rules.

3.2.1 Stage Load coefficient design rule

Between the compressor inlet and outlet, the Stage Loading Coefficient (SLC) indicates the amount of energy imparted to the flow through the specific stagnation enthalpy rise at each stage. Since specific stagnation enthalpy is known only at the compressor inlet and outlet, a SLC model is needed to suggest a feasible axial distribution of SLC at the compressor's design operating point. The maximum feasible specific static enthalpy rise in a stage Δh may be approximated by Equation (29) in Bullock and Prasse [94], with subscripts included for clarity.

$$\Delta h = \frac{2\sigma V_{REL.1} U_{WHEEL}}{J} \left(D + \frac{V_{REL.2}}{V_{REL.1}} - 1 \right) \quad (3.9)$$

The diffusion factor D is defined by Equation (13) in Lieblein et al. [95].

$$D = \left(1 - \frac{V_{REL.2}}{V_{REL.1}} \right) + \frac{\Delta V_\theta}{2\sigma V_{REL.1}} \quad (3.10)$$

where $\Delta V_\theta = |v_{REL.2} - v_{REL.1}|$ and $v = |\vec{v}|$.

In early compressors, Bullock and Prasse [94] reported that the compressor was also designed for reduced outlet axial velocity so that excessive or abrupt

deceleration before the combustor was avoided. This meant that the rear stages must use reduced axial velocities with smaller velocity triangles. The lower wheel speed would lead to smaller specific static enthalpy rises than the front stages. In recent combustor designs, the diffuser design incorporated after the combustor inlet has improved greatly, incurring acceptable stagnation pressure losses while slowing down the flow. This has removed the need for the compressor to produce greatly reduced axial speed for the combustor, which Mattingly et al. [9] demonstrated in the design approach for the combustor.

The RSRR compressor design approach in Mattingly [60], treats the diffusion factor, D as a design variable. This gives the designer greater flexibility to distribute SLC more evenly throughout the compressor and one feasible axial distribution of SLC is defining the specific stagnation enthalpy rise as a fixed proportion of $(U_{\text{WHEEL}})^2$, resulting in constant SLC.

The overall design of the engine is optimised for reduced cost and weight saving. The compressor is of no exception and therefore is likely close to the optimum least weight when finalised as Smith [59] points out. From his wealth of design experience, Smith [59] emphasizes the importance of loading each stage appropriately through advising designers and designs to work with proven loading criteria achievable through practical mechanical clearances.

When operating at a compressor's design point, the present study uses an equal or near equal distribution of SLC, with the following arguments.

- Each added stage increases weight and machine complexity such that the design must extract maximum useful output from any stage. Consequently, each stage's design applies the same utmost improvements in gained from aerodynamic insight.
- An individual stage may increase its pressure ratio through improved aerodynamic insight. Again, constraints on weight and on machine complexity demand the least number of stages. Therefore, each stage receives the same improved aerodynamic insight.
- Manufacturing challenges affect all stages almost consistently. Front or low-pressure (LP) stages use Variable Guide Vanes (VGV). Rear or high-pressure (HP) stages use integrated discs and compressor blades called blisks. Middle stages may use bleed valves. The compressor may run on double or triple concentric shafts for multi-spool designs. It is a reasonable argument that all stages incur similar manufacturing challenges and therefore, are subject to the same performance demands.
- While rear or HP stages could initially accept a lower SLC, weight and machine complexity constraints will still demand aerodynamic improvements to reduce non-optimised weight and machine complexity, for example the implementation of Outlet Guide Vanes (OGV) to remove swirl or improved diffuser designs in combustors to decelerate flow such that all stages are optimised. Similarly, when front or LP stages may initially use higher SLC with the implementation of IGVs, weight and machine complexity constraints demand that all stages improve.
- Stall and choke may occur at any stage. Sufficient stall margin and choke margin must be designed into each stage. Designing with constant SLC,

stage loading is proportional to available rotational kinetic energy. An equal SLC distribution may allow proportionally the same stall margin and choke margin to all stages.

- When no information is available, weight and machine complexity constraints do indicate that each stage shares the compression burden. IGV and OGV stages add and remove swirl respectively and must be present so the inlet stage and the outlet stage of the compressor are able to impart the same amount of work on the working fluid as the other stages as explained in Mattingly [60].

3.2.2 Pressure ratio design rule

While a compressor has a highly efficient design, there will be losses and specific entropy rises across each stage, arising from irreversibility in compression. Considering the need to minimize weight and complexity again, the relationship between the stage pressure ratios would be similar to that for SLC; each stage bears a similar burden. A feasible axial distribution of pressure ratios when operating at a compressor's design point is a near-equal distribution, dividing the overall pressure ratio into near-equal stage pressure ratios or near-equal diffusion processes for all stages.

Based on the compressor outlet's pressure rise and temperature rise, a corresponding overall specific entropy rise is known. After apportioning the compressor pressure rise and temperature rise nearly equally across all stages, each stage is able to see a small but unavoidable specific entropy rise.

3.2.3 Axial velocity design rule

For minimal buildup of wakes and boundary layers to maximise effective flow area for greater mass flow rates, Bullock and Prasse [94] point out the need to minimise abrupt changes at the component mating surfaces of the stage inlets and outlets. Implementing this guide, the casing and hub walls are made to vary smoothly from compressor inlet to outlet so that changes to the boundary layers and then wakes are gradual. The axial velocity distribution model depends on this resulting smoothly varying cross sectional areas and densities. The axial temperature and axial pressure distributions must therefore, return a density distribution that is varying smoothly. This results in a smooth variation of axial velocity for use in further analysis with velocity triangles.

3.2.4 Axial blockage design rule

Due to boundary layers and wakes accumulating from stage to stage, the effective flow area at each stage gradually decreases. While the blockage in the compressor increases, the ideal distribution must be smoothly changing so that the available flow area is able to give a smooth axial velocity profile. This works in tandem with Smith's [59] advice of removing all forward facing steps and obtaining surface finishes to appropriate smoothness. This study includes the effect of viscosity as an additional increase in blockage over mechanical blockage from the rotor and stator blades.

3.2.5 Velocity triangles design rule

At the design operating point, a compressor is performing at its ideal state aerodynamically. Following the advice of Smith [59], the blades are uniquely

designed for the design operating point. The working fluid follows the curvature of the blades with minimum deviations from the design intention. For minimum variation in flow angles between the exit plane of a blade row to the inlet plane of the next blade row, it would be a reasonable argument that the outlet velocity triangle of a blade row is the same or very similar to the inlet velocity triangle of the next blade row for the following reasons. This minimizes the onset of flow separation in the adverse pressure gradient on the suction side of each compressor blade and that in turn minimizes the onset of stall and maximizes diffusion taking place within adjacent blades to give maximum compressor efficiency. To begin solving for the stage inlet and outlet velocity triangles, the straightforward RSRR design guideline is used to initialise the design process. This initial design assumption results in similar flow angles at the stage inlet and outlet. As the compressor's design matures, the stage inlet and outlet flow angles variations are allowed.

In the LM2500 axial compressor, the axial velocity and the wheel speed are not constant throughout the compressor, implying varying velocity triangles. Attempting to obtain similar absolute velocity and relative velocity flow angles at the stage inlet and outlet is too stringent. Among the many possible departures from the RSRR design guide, the present study retained only the design rule of similar relative velocity flow angles at the stage inlet and outlet, until minor changes are necessary to achieve a converged set of flow angles for all blades in all stages.

3.2.6 Iteration variables

Ready with all the inputs in the categories listed above, there are still 2 unknown flow angles that influence the flow speeds within the compressor. As the IGV flow turning angle is unknown, the absolute inlet flow angle of the first stage is also unknown. The other unknown angle is the absolute outlet flow angle at the last stage of compressor before the OGV, which is also referred to as the absolute OGV inlet angle. These flow angles will be the iteration variables to explore the design space of flow angles for each stage. When a combination of IGV flow turning angle and absolute OGV inlet flow angle returns a set of flow angles, from all the stages, where the differences between inlet velocity triangles and outlet velocity triangles are acceptably small, this set of flow angles and their corresponding flow speeds is considered a converged solution of the stage un-stacking method.

3.2.7 Design guidelines for uncertain information

To reduce assuming a fixed value for uncertain information, the following guidelines are implemented:

1. The axial flow speed, outer radius and inner radius are varying smoothly in the axial direction to reduce boundary layer build up.
2. The stator and rotor blades are likely to have similar camber angles at the initial design stage. Since flow is more energetic across the rotor, the rotor blade is allowed more camber than the stator blade as the calculation progresses.
3. Stage reaction is initially assumed at 0.5 and is allowed to vary between 0.0 and 1.0.

4. The de Haller number is calculated at each stage and checked against the historical achievement of >0.72 , as used in Falck's [65] design approach. Saravanamuttoo et al. [96] discusses the de Haller number as only an initial design criterion. Due to the lack of more intimate machinery details in the present study, the de Haller number is sufficient for the stage un-stacking method. The diffusion factor is a detailed design criterion requiring further compressor details which may not be available.
5. The inlet velocity triangle of a stage is very similar to the outlet velocity triangle of the previous stage.

3.2.8 Stage un-stacking method overview

The stage un-stacking method is developed in 3 main parts: 1. Thermodynamic model, 2. Axial variation model, 3. Velocity triangle model. These models are deployed in the sequence in the flowchart of Figure 3.4. Parts 4 and 5 are used for convergence. This stage un-stacking method is implemented in the Python scripting language. Since an actual gas turbine fulfills simultaneous requirements, iterative calculations are used to match the flow quantities throughout the gas turbine. For parts 1-3 of the method, after 2 flow angles are selected as iteration variables and the remaining uncertain design variables are allowed to vary within acceptable bounds. Radial variation is not considered. The outputs from part 3 are used as input in a subsequent 3D CFD analysis of an approximated actual compressor to evaluate the method. The thesis sections related to each model is listed beside the flow chart.

Figure 3.4. Overview of the stage un-stacking method and related thesis sections

A non-converging attempt and its adjustment are recorded in section 4.1.5. The IGV flow turning angle is adjusted while all other settings or choices retained.

3.2.9 Stages without variable guide vanes (VGVs)

As greater compression takes place in the high pressure stages where there is typically no VGV, the SLC and flow angle relationship is examined next. At non-VGV stages, the angles of the velocity triangles at both the rotor inlet and the rotor outlet need to be fairly consistent across a range of rotational speeds, ω to

achieve the intended pressure rise. This implies at the inlet and outlet stations of a blade row, the ratio of absolute speed V_{ABS} : relative speed V_{REL} : wheel speed U_{WHEEL} in Figure 3.5 must remain similar to maintain velocity triangles of similar proportions when varying rotational speed.

Figure 3.5. Velocity diagram for the rotor inlet and rotor outlet

The Euler whirl equation, e_{WHIRL} is

$$e_{WHIRL} = \Delta h_{TOT.STG} = \omega r_2 |\vec{v}_2| - \omega r_1 |\vec{v}_1| \quad (3.11)$$

Combining the Euler whirl equation and SLC, ψ for an axial stage gives

$$\psi = \frac{\Delta h_{TOT.STG}}{|\vec{U}_{WHEEL}|^2} = \frac{\omega r_2 |\vec{v}_2| - \omega r_1 |\vec{v}_1|}{|\vec{U}_{WHEEL}|^2} \quad (3.12)$$

Defining wheel speed $|\vec{U}_{WHEEL}|$ at station 1 as $|\vec{U}_{WHEEL.1}|$,

$$\begin{aligned} \psi &= \frac{\omega r_2 |\vec{v}_2| - \omega r_1 |\vec{v}_1|}{|\vec{U}_{WHEEL.1}|^2} \\ &= \frac{\omega r_2 |\vec{v}_2|}{|\vec{U}_{WHEEL.1}|^2} - \frac{\omega r_1 |\vec{v}_1|}{|\vec{U}_{WHEEL.1}|^2} \end{aligned} \quad (3.13)$$

Using the wheel speeds at stations 1 and 2, and noting that ω is common since the same shaft is used,

$$\omega = \frac{|\vec{U}_{\text{WHEEL.1}}|}{r_1} = \frac{|\vec{U}_{\text{WHEEL.2}}|}{r_2} \quad (3.14)$$

a relationship between wheel speeds at different stations of varying radius is found

$$|\vec{U}_{\text{WHEEL.1}}| = \frac{r_1}{r_2} |\vec{U}_{\text{WHEEL.2}}| \quad (3.15)$$

SLC becomes

$$\begin{aligned} \psi &= \frac{r_2^2}{r_1^2} \frac{\omega r_2 |\vec{v}_2|}{|\vec{U}_{\text{WHEEL.2}}|^2} - \frac{\omega r_1 |\vec{v}_1|}{|\vec{U}_{\text{WHEEL.1}}|^2} \\ &= \frac{r_2^2}{r_1^2} \frac{|\vec{v}_2|}{|\vec{U}_{\text{WHEEL.2}}|} - \frac{|\vec{v}_1|}{|\vec{U}_{\text{WHEEL.1}}|} \end{aligned} \quad (3.16)$$

The components of absolute speed gives a relation between $|\vec{u}_1|$ and $|\vec{v}_1|$.

$$|\vec{u}_1| = |\vec{V}_{\text{ABS.1}}| \cos \alpha_1 = \frac{|\vec{v}_1|}{\tan \alpha_1} \quad (3.17)$$

The subsequent analysis is to relate $|\vec{v}_1|$ and $|\vec{U}_{\text{WHEEL.1}}|$ with both flow angles α and β . Using the two triangles in Figure 3.5, found above and below the axial velocity vector, the wheel speed, $|\vec{U}_{\text{WHEEL.1}}|$ is related to the axial speed, $|\vec{u}_1|$ by Equation (3.18).

$$\frac{|\vec{u}_1|}{|\vec{U}_{\text{WHEEL.1}}|} = \frac{1}{\tan \beta_1 + \tan \alpha_1} \quad (3.18)$$

Removing $|\vec{u}_1|$ and introducing $|\vec{v}_1|$ with Equation (3.17) at station 1 gives

$$\frac{|\vec{v}_1|}{|\vec{U}_{\text{WHEEL.1}}|} = \frac{\tan \alpha_1}{\tan \beta_1 + \tan \alpha_1} \quad (3.19)$$

Similarly, at station 2,

$$\frac{|\vec{v}_2|}{|\vec{U}_{\text{WHEEL.2}}|} = \frac{\tan \alpha_2}{\tan \beta_2 + \tan \alpha_2} \quad (3.20)$$

Returning to SLC in Equation (3.16), SLC becomes

$$\psi = \frac{r_2^2}{r_1^2} \frac{\tan \alpha_2}{\tan \beta_2 + \tan \alpha_2} - \frac{\tan \alpha_1}{\tan \beta_1 + \tan \alpha_1} \quad (3.21)$$

Within a non-VGV stage, Equation (3.21) indicates that SLC depends on the flow angles and the variation between r_1 and r_2 . Since in rear high pressure stages with no VGV capability, flow angles need to remain constant at varying rotational speed, ω , SLC is necessarily constant when varying ω at each non-VGV stage. However, there is no guidance for varying SLC between the stages.

3.2.10 Building a basic axial compressor

The compressor performance data from Pedersen [6] for the highest power output is the basis for inferring a possible design point for this axial compressor. The inferred design is further refined by examining the effects of various design rules implemented in the following sections. Within this stage un-stacking method, the actual determination of the blade metal angles and its use are avoided.

3.2.10.1 Blockage model

Blockage in a gas turbine compressor is challenging to define accurately due to the accumulation of wakes from multiple bodies interrupting the flow. Falck's [65] LUAX-C design code suggests that the blockage increases at 0.5% per stage and stabilises after stage 8. The final blockage is set to 10% based on data from

Pedersen [6]. Blockage models 1 and 2 suggest blockage increasing to a final value of 10% by stage 9 and remain constant thereafter. Blockage model 1 uses a smooth transition, while blockage model 2 uses an abrupt transition, both ending at stage 9. The data from Pedersen [6] indicates that the maximum available flow area through the compressor follows a steep “s” shaped curve and reaches a steady level of 90% of the available cross sectional area in the last few stages of the compressor and is designated as blockage model 3. All 3 blockage models are shown in Figure 3.6.

Figure 3.6. Blockage models in the present study

3.2.10.2 Thermodynamic model

As the inlet conditions of the compressor are not available, the inlet conditions are estimated at 100000 Pa and 278.15 K. At the compressor outlet, there is only information on stagnation temperature and static pressure. This information is transferred onto the OGV inlet, which is immediately after the last stator blade row. The outlet static temperature is determined at the OGV inlet instead, through iteration with the help of the estimated velocity components $\vec{u}$ and $\vec{v}$ (u and v). The orientation of $\vec{u}$ and $\vec{v}$ is shown in Figure 3.5.

$$u = \frac{\dot{m}}{\rho AB} \quad (3.22)$$

The Gas law gives density ρ as function of temperature and pressure. Viscosity and wakes buildup throughout the compressor, increasing blockage for the axial flow. The minimum blockage accumulated at the end of the compressor is 10.0%, based on the available flow area in Pedersen [6] and the blockage model then defines the blockage value B as 90%.

At the OGV inlet, v depends on the stator outlet flow angle, which is also an unavailable piece of information. However, v may be efficiently defined as a fraction, k_u of the wheel speed from Equation (3.14).

$$v = k_u \omega r_E \quad (3.23)$$

where r_E is the Eulerian radius at each blade row and $r_E = \sqrt{0.5(r_{\text{CASE}}^2 + r_{\text{CORE}}^2)}$. The outlet static temperature T is found through the outlet stagnation temperature, T_{TOT} .

$$T_{\text{TOT}} = T + \frac{1}{2c_p} (u^2 + v^2) \quad (3.24)$$

With OGV inlet temperature and pressure determined, the specific entropy rise in the whole compressor is calculated.

3.2.10.3 Inlet guide vane model

As the IGV is a flow device with no moving parts and only smooth, gently curving walls, the blockage estimated to accumulate at the end of the IGV is assumed as 1.00%, contributed mainly by the boundary layer growth. In comparison, from the same gas turbine manufacturer, Holloway et al. [69] report a blockage of 3% at the first rotor inlet when designing a highly loaded 10-stage axial compressor with an overall pressure ratio of 23 for aviation. With no further

information, a small 0.01% of the entire specific entropy rise is assumed to take place in the IGV, with the remainder through the compressor. The IGV is also assumed to incur no flow losses given its short length and smooth gradual flow-turning angle. The compressible Bernoulli in Equation (3.25) is one of the governing equations for the IGV, selected for its conservation of specific stagnation enthalpy.

$$\begin{aligned} \left(\frac{\gamma_1}{\gamma_1 - 1}\right) \frac{P_1}{\rho_1} + \frac{1}{2}(u_1^2 + v_1^2) \\ = \left(\frac{\gamma_2}{\gamma_2 - 1}\right) \frac{P_2}{\rho_2} + \frac{1}{2}(u_2^2 + v_2^2) + k_{LOSS} \frac{1}{2} u_1^2 \end{aligned} \quad (3.25)$$

Station 1 is the IGV inlet while station 2 is the IGV outlet. As the changes in elevation are very minor within the IGV, the gz term is omitted. The loss coefficient k_{LOSS} is assumed zero but should it be needed, the reference velocity is u_1 instead since this is the only known velocity and v_1 is zero at the inlet. The other governing equation is the second law of Thermodynamics, where specific entropy is determined as a function of temperature and pressure.

$$\Delta s_{IGV} = s_2 - s_1 = s_2(T_2, P_2) - s_1(T_1, P_1) \geq 0 \quad (3.26)$$

Due to flow turning, increasing rotational speed and maintaining mass flow rate, the kinetic energy increases at the expense of thermal energy and pressure through the IGV.

3.2.10.4 SLC model

In this stage un-stacking method, 4 possible SLC distribution models are suggested. Each model shapes the design SLC distribution, which is applied to temperature data from the design operating point (which outputs maximum power) to determine the stage temperatures. There is no preferred model as

each gas turbine has its unique heritage and possibly additional stages were designed differently as evident in the account by Smith [59] for a gas turbine manufacturer.

1. **Constant SLC for non-VGV stages and constant SLC for VGV stages.** The design SLC is the maximum SLC among all levels of power output. At each level of power output, the specific stagnation enthalpy rise through the compressor, $\Delta h_{TOT.COMP}$ with corresponding rotational speed ω is used in Equation (3.27) to determine the SLC, ψ .

$$\Delta h_{TOT.COMP} = \psi \omega^2 \sum_{STG=1}^{STG_{MAX}} r_{E.STG}^2 \quad (3.27)$$

Using the set of data from Pedersen [15] with 11 power output levels and thermodynamic data from Cengel [97], the third highest power output gives the largest ψ , which is the design SLC, ψ_{DS} . The thermodynamic data from Cengel [97] is divided into a few temperature ranges and curve fitted with different equations for each range, resulting in small discontinuities. Alternatively, with an air composition model, the thermodynamic data for air may be calculated with polynomial functions of temperature such as by McBride et al. [98].

2. **Constant temperature-rise for all stages.** Based on the highest power output, Equation (3.28) gives the temperature at each stage outlet. The velocity at the mean line fixes the specific stage stagnation enthalpy in Equation (3.29) and in turn, determines the design SLC for each stage, $\psi_{DS.STG}$.

$$T_{\text{STG.OUT}} = T_{\text{COMP.IN}} + (\text{STG}) \frac{\Delta T_{\text{COMP}}}{\text{STG}_{\text{MAX}}} \quad (3.28)$$

$$h_{\text{TOT.STG.OUT}} = h(T_{\text{STG.OUT}}) + \frac{1}{2}(u_{\text{STG}}^2 + v_{\text{STG}}^2) \quad (3.29)$$

This SLC model which is based on constant temperature rise through all stages is inspired by a worked example in Mattingly [60], where a preliminary compressor is designed. Without detailed stage temperature information, this suggestion is reasonable.

3. **Constant specific static enthalpy rise for all stages.** Using the operating point with the highest power output, Equation (3.30) calculates the specific stagnation enthalpy at each stage outlet, which in turn determines the design SLC for each stage, $\psi_{\text{DS.STG}}$.

$$h_{\text{TOT.STG.OUT}} = h_{\text{COMP.IN}} + (\text{STG}) \frac{\Delta h_{\text{COMP}}}{(\text{STG}_{\text{MAX}})} + \frac{1}{2}(u_{\text{STG}}^2 + v_{\text{STG}}^2) \quad (3.30)$$

The form of the SLC model based on constant specific static enthalpy rise shares the same inspiration as the constant temperature rise SLC model and supported by a rule of thumb for constant stage energy rise in [99]. Specific static enthalpy is the variable as this is also common in turbomachinery analysis.

4. **Varying (decreasing) SLC across the stages.** The SLC at the last stage is a percentage lower than the SLC at the first stage, with SLC varying linearly across all the middle stages. Using the operating point with the highest power output, Equation (3.31) gives the specific stage stagnation enthalpy rise in terms of the design SLC of each stage, $\psi_{\text{DS.STG}}$. Using the specific

stagnation enthalpy rise for the full compressor, Equation (3.32) determines the design SLC of each stage.

$$\Delta h_{\text{TOT.STG}} = \psi_{\text{DS.STG}} (\omega r_{\text{E.STG}})^2 \quad (3.31)$$

$$\Delta h_{\text{TOT.COMP}} = \sum_{\text{STG}=1}^{\text{STG}_{\text{MAX}}} \Delta h_{\text{TOT.STG}} \quad (3.32)$$

This decreasing SLC model was inspired by [68] where the front stages are deliberately highly loaded.

To determine the stage load coefficient, the axial and rotational components of the absolute velocity must be available. However, these are only found after analysis with velocity triangles. This indicates that a more comprehensive solution requires iteration. To test the robustness of the solution procedure, the SLC in Equation (3.12) is approximated by arguing that the specific stage stagnation enthalpy rise is similar to the specific stage static enthalpy rise, $\Delta h_{\text{TOT.STG}} \approx \Delta h_{\text{STG}}$ and this removes the need to iterate as Δh_{STG} may be determined without velocity inputs.

3.2.10.5 Pressure ratio model

In this stage un-stacking method, 3 possible pressure ratio models are suggested, each built with an efficiency model and a specific entropy model. Each pressure ratio model suggests a feasible relative distribution of stage pressure ratios across all the stages. There is no best model as pressure ratio is determined stage by stage to meet the overall pressure ratio, which in turn fulfills several possible objectives. The gas turbine could have been designed for maximum overall pressure ratio at acceptable efficiency, maximum efficiency

at acceptable overall pressure ratio or the most economical maintenance package. An inference using the overall pressure ratio is at best an estimate and cannot compensate for unavailable information, considering that an actual design has as much as a million details as pointed out by Ghisu et al. [54].

1. **Pressure ratio guided by small stage polytrophic efficiency using reference specific entropy (function of temperature)**
2. **Pressure ratio guided by small stage polytrophic efficiency using specific entropy (function of temperature, pressure)**
3. **Pressure ratio guided by fully isentropic compression based specific entropy (function of temperature, pressure)**

In pressure ratio model 1, the actual specific stage entropy rise is not known beforehand. However, the stage efficiency may be approximated by the compressor's polytrophic efficiency according to Equation (3.33), with a mean γ , $\bar{\gamma}$ determined from the conditions at the inlet and outlet of the compressor.

$$\eta_{\text{STG}} = \frac{h_{2i} - h_1}{h_2 - h_1} = \eta_{\text{POLY}} \quad (3.33)$$

$$= \frac{\bar{\gamma} - 1}{\bar{\gamma}} \frac{\ln(P_2/P_1)}{\ln\left\{\left(1/\eta_{\text{COMP}}\right)\left[(P_2/P_1)^{(\bar{\gamma}-1)/\bar{\gamma}} - 1\right] + 1\right\}}$$

The specific stage outlet static enthalpy, h_2 and the specific stage isentropic outlet static enthalpy, h_{2i} lie on the same isobar on the $h - s$ diagram, experiencing the same pressure rise. To avoid the still unknown actual specific stage entropy rise, isentropic compression calculation is carried out with h_{2i} . The specific entropy rise in Equation (3.34) is set to zero and using $T_{2i} = T(h_{2i})$, a feasible stage pressure ratio is estimated from P_2/P_1 .

$$\Delta s_{\text{STG}} = s_0(T_{2i}) - s_0(T_1) - R \ln \frac{P_2}{P_1} = 0 \quad (3.34)$$

The specific reference entropy, s_0 is from the thermodynamic table for air from Cengel [97].

Pressure ratio model 2 is similar to pressure ratio model 1 except specific entropy is a function of temperature and pressure based on the s - T - P chart by Aartun [100]. Using the stage inlet temperature, T_1 and the stage isentropic outlet temperature, T_{2i} the specific entropy rise in Equation (3.35) determines the stage pressure ratio, P_2/P_1 .

$$\Delta s_{\text{STG}} = s(T_{2i}, P_2) - s(T_1, P_1) = 0 \quad (3.35)$$

In pressure ratio model 3, knowing that for a given temperature rise, $T_2 - T_1$ the maximum pressure rise occurs when the specific entropy rise is zero. With available inlet and outlet temperatures from the selected SLC model, specific entropy is found as a function of temperature and pressure based on the s - T - P chart by Aartun [100]. Equation (3.36) determines the maximum stage pressure ratio, P_2/P_1 .

$$\Delta s_{\text{STG}} = s(T_2, P_2) - s(T_1, P_1) = 0 \quad (3.36)$$

The actual stage pressure ratio is lower than maximum stage pressure ratio, and in this way, accounts for the specific stage entropy rise. The specific stage entropy rise is proportional to the maximum pressure rise in a stage for the same stage efficiency and assuming nearly linear isobars on the T - s diagram. In this way, the stage losses are distributed according to the stage compression capability.

3.2.10.6 Method of smoothing the axial velocity variation

The actual pressure ratio is a fraction of the relative distribution of stage pressure ratios found earlier and is determined such that a smooth axial velocity distribution results. All stages are subjected to the same fraction except the first stage. In the LM2500 axial compressor, the same fraction k_{PR} is applied on stages 2 to 16 and $k_{PR,1}$ for stage 1. The iteration variable is k_{PR} . Each guessed k_{PR} is automatically constrained by Equation (3.37) such that all stage pressure ratios achieve the overall pressure ratio of the compressor, OPR as $k_{PR,1}$ takes the slack.

$$OPR = PR_{ACT,1} \prod_{STG=2}^{STG_{MAX}} PR_{ACT,STG} \quad (3.37)$$

where $PR_{ACT,STG} = k_{PR} PR_{MOD,STG}$ and $PR_{ACT,1} = k_{PR,1} PR_{MOD,1}$.

Next, the stage temperature, Gas law and mass flow rate conservation determine the no-blockage axial velocity at each stage outlet. Iteration continues till the no-blockage velocity distribution from stage 1 to stage 3 varies linearly with compressor axial coordinate x , in a straight line fit of 3 points. The no-blockage velocity was selected as it depends only on geometry since the boundary layer build up is assumed small at the beginning of the compressor.

3.2.10.7 Velocity triangle model

The velocity triangles of the last stage of this compressor are determined first since at the outlet of the last stage, all the flow quantities are known. In the analysis of stages without VGVs, such stages require similar velocity triangles, which in turn need similar SLC values. Solving from the last stage to the first

stage results in more similar flow angles in the last stages as departures from the RSRR design guide are admitted only at the front stages. This approach seems able to determine a complete set of flow angles for all stage with lesser difficulties.

For each stage, the solution is a set of blade angles and flow angles where the Euler whirl matches the specific stagnation enthalpy rise, where the de Haller number is met for both rotor and stator and the stage reaction is reasonable. The stage reaction is initially 0.5 and allowed to vary as iteration proceeds. The rotor blade is given more curvature than the stator blade as the solution iterates.

At each stage, the solution process begins at the stage outlet, where specific stagnation enthalpy, the flow velocities, blade angles and thermodynamic properties are found. Moving to the stage inlet, this stage un-stacking method applies only initially the design rule of similar relative velocity flow angles at the stage inlet and outlet, $\beta_1 = \beta_3$. The β_1 angle enables determining the stage inlet flow angles, blade angles and thermodynamic properties. The rotor-stator interface quantities in the middle of the stage are determined by degree of reaction, R_{REACT} in Equation (3.38),

$$h_2 = h_1 + R_{\text{REACT}}(h_3 - h_1) \quad (3.38)$$

and conservation of specific stagnation enthalpy across stator in Equation (3.39). This sets up the specific static enthalpy and specific stagnation enthalpy to determine the absolute velocity.

$$h_{\text{TOT.2}} = h_{\text{TOT.3}} \quad (3.39)$$

Using the absolute velocity, the rotor-stator interface blade angles and thermodynamic properties are found. With all flow angles and thermodynamic properties available, the stage Euler whirl in Equation (3.11) is the “hard” criteria used to test the suitability of stage reaction and inlet relative velocity angle. The first “soft” criterion is the stage degree of Reaction, which ranges about 0.5 for the axial compressor in the present study. The next “soft” criteria is the difference in blade angles, $\Delta\theta$ from blade angles, $\theta_{\text{ROT}} = \beta_1 - \beta_2$ and $\theta_{\text{STA}} = \alpha_3 - \alpha_2$.

$$\Delta\theta = \theta_{\text{ROT}} - \theta_{\text{STA}} \quad (3.40)$$

The de Haller number, $d\mathcal{H}$ is the last “soft” criteria, which is a ratio of relative outlet speed to relative inlet speed for the rotor blades and absolute outlet speed to absolute inlet speed for the stator blades.

$$d\mathcal{H}_{\text{ROT}} = V_{\text{REL.2}}/V_{\text{REL.1}} \quad (3.41)$$

$$d\mathcal{H}_{\text{STA}} = V_{\text{ABS.3}}/V_{\text{ABS.2}} \quad (3.42)$$

Since there is insufficient design information to allow a direct calculation of the flow and blade angles, a suitable range of values are accepted for the design variables, R_{REACT} , $\Delta\theta$ are $d\mathcal{H}$. Being a “hard” criteria, Euler whirl, e_{WHIRL} is used in an error variable $\varepsilon_{\text{HARD}}$ in Equation (3.43) to iteratively suggest a $\Delta\theta$ that results in an Euler whirl that matches the specific stage stagnation enthalpy rise.

$$\varepsilon_{\text{HARD}} = \frac{e_{\text{WHIRL}} - (h_{\text{TOT.3}} - h_{\text{TOT.1}})}{h_{\text{TOT.3}} - h_{\text{TOT.1}}} \quad (3.43)$$

Consequently, the stage degree of reaction is also affected and is updated with another error variable $\varepsilon_{\text{SOFT}}$ in Equation (3.44).

$$\varepsilon_{\text{SOFT}} = \frac{\theta_{\text{ROT}} - (\theta_{\text{STA}} + \Delta\theta)}{\theta_{\text{STA}} + \Delta\theta} \quad (3.44)$$

When the stage degree of reaction and acceptable angle difference $\Delta\theta$ between the rotor and stator blade angles do not result in feasible set of blade and flow angles, the inlet relative flow angle β_1 is adjusted with the $\varepsilon_{\text{HARD}}$ error variable. The design variables V_{DS} are updated with their error variables ε and a relaxation factor, f_{RELAX} to prevent over-correction, according to Equation (3.45).

$$V_{DS.\text{NEW}} = V_{DS.\text{OLD}}(1 \pm f_{\text{RELAX}}\varepsilon) \quad (3.45)$$

where the subscripts “NEW” and “OLD” refer to the updated and previous values respectively.

3.3 Transport Equations in the present study

The following transport equations are used in the present study for the 3D simulation of the LM2500 axial compressor and the 2D simulation of Smyth and Bryner’s experiment of flammable gas flowing past a heated foil.

Mass balance

$$\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot (\rho \vec{u}) \quad (3.46)$$

Momentum balance

$$\rho \frac{\partial \vec{u}}{\partial t} = -\rho \vec{u} \vec{\nabla} \cdot \vec{u} - \vec{\nabla} \cdot (P\mathbf{I} + \tau) + \rho \vec{g} \quad (3.47)$$

Total energy balance

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho e) + \underbrace{\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\vec{u}^2\right)}_{\text{ME}} + \underbrace{\frac{\partial}{\partial t}(\rho\psi)}_{\text{PE}} \\
& = -\vec{\nabla} \cdot (\rho e \vec{u}) - \underbrace{\vec{\nabla} \cdot \left(\frac{1}{2}\rho\vec{u}\vec{u}^2\right)}_{\text{ME}} - \underbrace{\vec{\nabla} \cdot (\rho\psi\vec{u})}_{\text{PE}} - \underbrace{\vec{u}\vec{\nabla} \cdot (PI + \tau)}_{\text{ME}} \\
& \quad - (PI + \tau)\vec{\nabla} \cdot \vec{u} - \vec{\nabla} \cdot q + \dot{q}_{\text{RAD}} + \underbrace{\rho\vec{u} \cdot \vec{g}}_{\text{ME}} - \underbrace{\rho\vec{g} \cdot \vec{u}}_{\text{PE}}
\end{aligned} \tag{3.48}$$

where “ME” and “PE” refer to mechanical and potential energy respectively.

Enthalpy balance with the transient pressure term and without radiation

$$\frac{\partial}{\partial t}(\rho h) + \vec{\nabla} \cdot (\rho h \vec{u}) = -\tau \vec{\nabla} \cdot \vec{u} - \vec{\nabla} \cdot q + \frac{\partial P}{\partial t} + \vec{u} \cdot \vec{\nabla} P \tag{3.49}$$

Turbulent momentum balance

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho \bar{u}_i) + \frac{\partial}{\partial x_i}(\rho \bar{u}_i \bar{u}_j) \\
& = -\frac{\partial P'}{\partial x_i} + \underbrace{\frac{\partial}{\partial x_i} \left[(\mu + \mu_{\text{TURB}}) \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right]}_{\text{diffusion term}} + S_M
\end{aligned} \tag{3.50}$$

Turbulent total enthalpy balance with the transient pressure term and without radiation

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho \bar{h}_{\text{TOT}}) - \frac{\partial P}{\partial t} + \frac{\partial}{\partial x_i}(\rho \bar{u}_i \bar{h}_{\text{TOT}}) \\
& = \underbrace{\frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} + \frac{\mu_{\text{TURB}}}{Pr_{\text{TURB}}} \frac{\partial h}{\partial x_i} \right)}_{\text{diffusion term}} + \frac{\partial}{\partial x_i} [\bar{u}_i (\tau_{ij} - \rho \bar{u}_i \bar{u}_j)] + S_E
\end{aligned} \tag{3.51}$$

Turbulent chemical species mass fraction balance

$$\frac{\partial}{\partial t}(\rho \bar{Y}_I) + \frac{\partial}{\partial x_i}(\rho \bar{u}_i \bar{Y}_I) = \underbrace{\frac{\partial}{\partial x_i} \left[\left(\Gamma_I + \frac{\mu_{\text{TURB}}}{Pr_{\text{TURB}}} \right) \frac{\partial \bar{Y}_I}{\partial x_i} \right]}_{\text{diffusion term}} + S_{Y_I} \tag{3.52}$$

Since the focus is the simulation of heat transfer from the heated foil surface to the flowing flammable methane and air mixture, the basic turbulence model used is the baseline (BSL) k - ω SST model in Equations (3.53) and (3.54). The contribution of buoyancy to turbulence is included through the production terms $P_{k,BUO}$ and $P_{\omega,BUO}$.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) \\ = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_{TURB}}{\sigma_{k3}} \right) \frac{\partial k}{\partial x_i} \right] + P_k - \beta' \rho k \omega + P_{k,BUO} \end{aligned} \quad (3.53)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho u_i \omega) \\ = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_{TURB}}{\sigma_{\omega 3}} \right) \frac{\partial \omega}{\partial x_i} \right] + (1 - F_1) 2\rho \frac{1}{\sigma_{\omega 2} \omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i} \\ + \underbrace{\alpha_3 \frac{\omega}{k} P_k}_{\omega \text{ source}} - \beta_3 \rho \omega^2 + P_{\omega,BUO} \end{aligned} \quad (3.54)$$

The coefficients σ_{k3} , $\sigma_{\omega 3}$, α_3 and β_3 are a linear combination of coefficients from the Wilcox turbulence model and transformed k - ε turbulence model. F_1 is a blending function in the BSL k - ω turbulence model.

To focus on the effect of turbulence, the k - ω SST-sustain turbulence model from Rumsey [101] is also considered. The ambient k_{AMB} and ω_{AMB} are the initial ambient k and ω . The transport equations are

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho u_i k) \\
&= \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_{\text{TURB}}}{\sigma_{k3}} \right) \frac{\partial k}{\partial x_i} \right] + P_k - \beta' \rho k \omega + P_{k,\text{BUO}} \\
&+ \beta' \rho k_{\text{AMB}} \omega_{\text{AMB}}
\end{aligned} \tag{3.55}$$

And

$$\begin{aligned}
& \frac{\partial}{\partial t}(\rho \omega) + \frac{\partial}{\partial x_i}(\rho u_i \omega) \\
&= \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_{\text{TURB}}}{\sigma_{\omega 3}} \right) \frac{\partial \omega}{\partial x_i} \right] + (1 - F_1) 2\rho \frac{1}{\sigma_{\omega 2} \omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i} \\
&+ \underbrace{\frac{\alpha_3}{\nu_t} P_k}_{\omega \text{ source}} - \beta_3 \rho \omega^2 + P_{\omega,\text{BUO}} + \beta_3 \rho \omega_{\text{AMB}}^2
\end{aligned} \tag{3.56}$$

3.4 A first approach to hot surface ignition by numerical modelling

The previous sections cover methods that define the flow environment within the axial compressor, where ignition might take place. The ignition criterion in this section builds on the work of Pedersen et al. [79]. A reduced chemistry model that progresses according to Arrhenius rate parameters replaces the first and third part of their ignition criterion. The second part of their ignition criterion, the Van't Hoff criterion, is retained. The use of a reduced chemistry model enables a slightly closer study of the way finite rate chemistry determines the conditions for ignition, which in turn influence flammability limits and time leading to ignition.

In the present study, fluid flow is simulated together with finite rate chemistry Arrhenius model to represent the combustion process. The parameters of the

Arrhenius model are from Westbrook and Dryer [102], [17]. The combustion chemistry is summarized as a 2-step reaction mechanism, trading off model complexity for longer simulation time with smaller time steps. While a highly reactive 2-step reaction mechanism may not pin point a more correct ignition temperature, the identified ignition temperatures (1300 K to 1310 K) are sufficiently far from the temperatures found in the LM2500 axial compressor last stage (723 K). Therefore, this chemistry model is sufficient for concluding the role hot surface ignition.

The fluid and chemistry aspects are validated against Smyth and Bryner's [1] experimental result. While the low speed flow makes this seem like a laminar flow experiment, once combustion take place, the flow field is turbulent. Therefore, mildly turbulent transient simulations are used.

3.4.1 Problem definition for hot surface ignition

This study uses the software ANSYS CFX releases 14.5 through 19.1 in academic versions. CFX provides the flow environment for determining the onset of ignition. The available auto ignition model in CFX is targeted to predict ignition of flammable gas when the gas in the flow domain is above the AIT and hence incorporates only a time delay as a function of concentrations and temperature. This auto ignition model works with reacting mixtures and it suppresses ignition for infinitely fast reactions or prescribes ignition for reaction models that do not self-start. The onset of ignition is time based and τ_{IGN} may be user-defined as

$$\tau_{IGN} = B \exp(E_a/RT) [Fuel]^C [Oxidiser]^D \quad (3.57)$$

where B is a pre-exponent, E_a is the activation energy, C is the fuel concentration exponent and D is the oxidiser concentration exponent. Ignition is just a matter of time delay. For this reason, the available auto ignition model in CFX is unsuitable for the situation considered in the present study, as here the flammable gas is initially below its AIT.

In the present study, the ignition phenomenon is different. Here the initial flammable gas temperature is below its AIT, but the wall with which the mixture is in contact, has a temperature exceeding the AIT of the gas. Hence, due to the balance of heat transfer between the gas heating up, heat transport into the core gas flow and chemical reaction kinetics, the instant of ignition is determined. For that reason, a new approach that models the balance between these processes is developed.

As a start for the modelling of the processes mentioned above, a simple model is used to describe the chemical reactions including chemical kinetics. In order to avoid the increased computational cost of simulating with detailed chemical reaction chemistry, a 2-step reaction is used to describe the low temperature chemistry driven by the heat transfer from the hot surface into the gas mixture.

3.4.2 Adiabatic flame temperature

The target adiabatic flame temperatures are computed by CERFACS's adiabatic flame temperature online calculator [103] on the basis of chemical equilibrium using the species and Gibbs potentials of the GRI-Mech 3.0 [83]. The input parameters are pressure, equivalence ratio, initial temperature, fuel

and air composition. Initial temperatures from 1200 K to 1400 K are used. At each initial temperature, the equivalence ratio 0.7 is used. The overall pressure is constant at 1 atm. The fuel is only methane. The air model uses a 3.75 molar ratio of nitrogen to oxygen. Adiabatic flame temperatures relevant to the present study range from 2446 K to 2552 K.

3.4.3 An air composition model

The air composition model in the present study has 3 chemical species, nitrogen, oxygen and argon. The constraints are argon occupies a fixed 1.0% mole fraction and the molar ratio of nitrogen to oxygen is 3.75. After adding methane, the mole fractions are adjusted to give a mixture of desired equivalence ratio. The mole and mass fractions in a mixture with equivalence ratio 0.7 are recorded in Table 3.2.

Table 3.2. Mass and mass fractions of an equivalence ratio 0.7 methane-air mixture

Chemical species I	Molar mass M_I [g mol ⁻¹]	Mass m_I [g]	Mass fraction Y_I []
N_2	28.0134 [104]	20.392	0.72587
O_2	31.9988 [105]	6.2115	0.22111
CH_4	16.0425 [106]	1.0899	0.03880
Ar	39.9480 [107]	0.3995	0.01422
sums		28.092	1.00000

3.4.4 A 2-step reaction mechanism with Arrhenius rate equation

A 2-step reaction mechanism reported by Westbrook and Dryer [17] is used for its capability to output suitable adiabatic flame temperatures for the range of temperatures and equivalence ratios of interest in the present study. Based on the sequential burning of typical hydrocarbons, this 2-step mechanism is constructed from the Dryer and Glassman modification of the 1-step reaction for the oxidation of methane in a reactor with turbulent flow. In step 1, the methane

and oxygen react to form carbon monoxide and water. In step 2, carbon monoxide and oxygen react in a reversible reaction to produce carbon dioxide.

The step 1 reaction is

Two sets of Arrhenius parameters are taken from Table IV of Westbrook and Dryer [17] and reproduced in Table 3.3.

Table 3.3. Step 1 reaction parameters from Westbrook and Dryer [17]

Set	Pre-exponent A [depending]	Temperature exponent β []	Activation energy E_a [J mol ⁻¹]	Fuel exponent C []	Oxidiser exponent D []
MILD2	$1.5 \times 10^7 \text{ s}^{-1}$	0	125520.0	-0.3	1.3
VIGR2	$2.8 \times 10^9 \text{ s}^{-1}$	0	202505.6	-0.3	1.3

The negative fuel exponent poses a minor mathematical inconvenience, as fuel concentrations approach zero; it causes excessively high reactions rates. Westbrook and Dryer [17] suggest a few solutions such as setting a minimum concentration or using an alternative set of fuel and oxidizer exponents.

The improved form for $[CH_4]$ is $\max([CH_4], smc)$, where $smc = 1.0 \times 10^{-15} \text{ mol m}^{-3}$. An alternative concentration contribution, using an alternative set of fuel and oxidizer exponents, is $2.6\{\max([CH_4], smc)\}^{0.3}[O_2]^{0.7}$, where the exponents sum to 1.0 as in the original and preserves the units of the pre-exponent term. The factor 2.6 blends the original concentration contribution smoothly with the alternative concentration contribution when $[CH_4]$ drops before rising asymptotically as seen in Figure 3.7. The improvement takes the form $\min(\{\max([CH_4], smc)\}^{-0.3}[O_2]^{1.3}, 2.6\{\max([CH_4], smc)\}^{0.3}[O_2]^{0.7})$, which gives a meaning small reaction rate as $[CH_4]$ approaches zero. This improved

concentration contribution also allows slightly larger time steps, since the asymptotically large concentration contribution to the reaction rate is not use in further calculations.

Figure 3.7. Blending the original and alternative concentration contribution

The next challenge is when the available $[CH_4]$ is less than what the reaction rate expects to consume. A continuing condition cc_1 is introduced to check that sufficient $[CH_4]$ is available; else, the reduced reaction rate $[CH_4]/\Delta t$ is used.

$$cc_1 = \begin{cases} \text{true} & , [CH_4] > \Delta t \times bRR_1 \\ \text{false} & , [CH_4] \leq \Delta t \times bRR_1 \end{cases} \quad (3.59)$$

Considering the lower flammability limits of methane, the step 1 reaction proceeds only when $[CH_4] > smc$. The reaction rate of step 1 is RR_1 with the improvements mentioned above.

$$RR_1 = \begin{cases} AT^\beta \exp(-E_a/RT)[CH_4]^c [O_2]^D, & cc_1 = \text{true} \\ [CH_4]/\Delta t & , cc_1 = \text{false} \end{cases} \quad (3.60)$$

The step 2 reaction is

The parameters are from Westbrook and Dryer [17] and reproduced in Table 3.4.

Table 3.4. Step 2 reaction parameters Westbrook and Dryer [17]

Set	Pre-exponent A [depending]	Temp. exponent β []	Activation energy E_a [J mol ⁻¹]	Fuel exponent C []	Oxidiser exponent D []	Water exponent H []
FWD	$1.26 \times 10^{10} \text{ s}^{-1} \text{ mol}^{0.75} \text{ m}^{2.25}$	0	167360.0	1.0	0.25	0.5
BWD	$5.0 \times 10^8 \text{ s}^{-1}$	0	167360.0	1.0	-	-

Again, a pair of continuing condition $cc_{2,\text{FWD}}$ and $cc_{2,\text{BWD}}$ is introduced to check that sufficient $[CO]$ and $[CO_2]$ is available. When the reaction rates suggest a consumption that exceeds the available $[CO]$ or $[CO_2]$, the reduced forward reaction rate $[CO]/\Delta t$ or reduced backward reaction rate $[CO_2]/\Delta t$ is used. The continuing condition $cc_{2,\text{FWD}}$ for the forward reaction of step 2 is

$$cc_{2,\text{FWD}} = \begin{cases} \text{true} & , [CO] > \Delta t \times bRR_{2,\text{FWD}} \\ \text{false} & , [CO] \leq \Delta t \times bRR_{2,\text{FWD}} \end{cases} \quad (3.62)$$

The continuing condition for the backward reaction of step 2 is

$$cc_{2,\text{BWD}} = \begin{cases} \text{true} & , [CO_2] > \Delta t \times bRR_{2,\text{BWD}} \\ \text{false} & , [CO_2] \leq \Delta t \times bRR_{2,\text{BWD}} \end{cases} \quad (3.63)$$

Since there are only positive concentration exponents in the forward reaction rate, extremely small concentration values will not asymptotically drive up the reaction rates. The forward reaction rate in step 2, $RR_{2,\text{FWD}}$ is

$$RR_{2,\text{FWD}} = \begin{cases} AT^\beta \exp(-E_a/RT) [CO]^C [O_2]^D [H_2O]^H & , cc_{2,\text{FWD}} = \text{true} \\ [CO]/\Delta t & , cc_{2,\text{FWD}} = \text{false} \end{cases} \quad (3.64)$$

and the backward reaction rate in step 2, $RR_{2,\text{BWD}}$ is

$$RR_{2,\text{BWD}} = \begin{cases} AT^\beta \exp(-E_a/RT) [CO_2]^C & , cc_{2,\text{BWD}} = \text{true} \\ [CO_2]/\Delta t & , cc_{2,\text{BWD}} = \text{false} \end{cases} \quad (3.65)$$

3.4.4.1 Varying the reaction rate of step 1

For step 1 of the 2-step reaction, there are 2 sets of reaction rates: VIGR2 and MILD2. The VIGR2 set has a larger activation energy, starting out slow and

delaying the rapid temperature rise until a higher temperature but once that takes, place the reaction proceeds rapidly. The MILD2 set operates in the opposite manner. Both sets of reaction parameters give very similar features during ignition: a delay followed by a rapid temperature rise. These 2 sets of reaction rates may be combined to adjust the overall reaction rate to match known ignition delays. The reaction proportion r_p is introduced to combine contributions from both reactions using Equation (3.66).

$$RR_1 = r_p \times RR_{1,VIGR2} + (1 - r_p) \times RR_{1,MILD2} \quad (3.66)$$

3.4.5 Sources of turbulence intensity at the far field boundaries

At the far field boundaries in this present study, turbulence quantities are specified at the boundaries with “zero gradient” setting in CFX.

3.4.6 Sources of turbulence intensity at the Inlet flow

At the same time, in addition to these far field conditions, the inlet pipe below the plate is a source of the turbulence in the domain. The turbulence intensity is sought by considering a low speed fully developed turbulent flow in a smooth pipe and from measurements of air speed under low Reynolds number laminar flow conditions.

3.4.6.1 Low speed fully developed turbulent flow

The turbulence intensity of pipe flow is investigated semi-empirically, computationally and experimentally as a function of Reynolds number by Russo and Basse [108]. The measured radial velocity profiles are obtained experimentally from straight pipe flows with Reynolds number 8.13×10^4 to

5.98×10^6 . The radial velocity profiles of these fully developed turbulent compressible flows in a pipe are fitted with a semi-empirical model from Gersten [109], achieving agreement from the pipe axis to almost at the wall with a maximum variation of ± 1.0 %.

Scaling laws for turbulence intensity are fitted to measurements of turbulence intensity in the same set of fully developed turbulent compressible flows in a pipe where the Mach number is less than 0.1 [108]. The measurements of turbulence intensity from the pipe axis to the wall show turbulence intensity rising gradually and peaking just before the walls as seen in Figure 21 of [108]. From Figure 21 of [108], the slowest flow measurements are taken at $Re = 8.13 \times 10^4$. Using the standard Reynolds number definition $Re = \rho u d / \mu$ and the coefficients from Table 7 in [108], the following scaling laws based on compressible flow measurements are developed. At the pipe axis,

$$I_{CMPAxis} = 0.0550 Re^{-0.0407} \quad (3.67)$$

and averaging across the pipe area,

$$I_{CMPArea} = 0.2270 Re^{-0.1000} \quad (3.68)$$

where “CMPAxis” is “Compressible measurements, pipe axis” and “CMPArea” “Compressible measurements, pipe area”.

Turbulence intensity averaged across the pipe area is higher than turbulence intensity measured only at the pipe axis. Since the present study requires the effect of turbulence, even while under the laminar regime, the selected scaling law is the one that gives higher turbulence intensity, I_{TURB} .

$$I_{TURB} = \max(I_{CMPAxis}, I_{CMPArea}) \quad (3.69)$$

These scaling laws asymptotically increase near Reynolds number of zero, more so for I_{CMPArea} . Using the formulas for compressible pipe flow, where Reynolds number is 114.86 and mean velocity is 0.16 m s^{-1} , the turbulence intensity is $I_{\text{CMPAxis}} = 0.0453$ and $I_{\text{CMPArea}} = 0.141$.

3.4.6.2 Low Reynolds number laminar flow

A method is devised by Zou and Malmström [110] to obtain a fully developed laminar flow exiting a long straight tube. They make use of water entering an airtight container which in turn pushes air out through the long straight tube. The flowing air at the outlet of the long tube is used to calibrate a hot wire anemometer. The tube diameter is 0.013 m, and the steady state speed in the tube is 1 m s^{-1} . As no air temperature is given in [110], the temperature is assumed to be 295K, which is reasonable considering the measurement is taken indoors. This results in $Re = 848.41$, which is laminar. The turbulence level or turbulent intensity when the hot wire output voltage became steady was less than 0.4%. The overall uncertainty for all the other instruments used is $\pm 1.5\%$. The uncertainty of the hot wire anemometer is not mentioned.

3.4.6.3 Selected turbulence intensity

The flow conditions at the pipe outlet are $U_{\infty} = 0.16 \text{ m s}^{-1}$, $d_{\text{HYD}} = 0.011 \text{ m}$. The Reynolds number is 114.86 at 295 K. Using these inputs, this flow is laminar. The low Reynolds number laminar flow scenario referred to above has a similar diameter but about 6 times faster speed and results in a measured turbulent intensity $I_{\text{TURB}} = 0.004$. As speed reduces, it is reasonable to expect turbulent intensity to reduce but since no further information is available for the relation of

turbulent intensity to speed and that at zero mean speed minute turbulent fluctuations persist, the turbulent intensity is assumed to be constant for the speed range 0 to 1 m s⁻¹.

Just for comparison and assuming turbulent pipe flow where the I_{TURB} correlation is equally valid, the turbulent variables determined with Equation (3.67) give $I_{\text{TURB}} = 0.0453$. However to include the effect of turbulence on ignition, the turbulence level in the turbulent simulations are set at $I_{\text{TURB}} = 0.05$, which is a default value in the CFX and also close to the outcome of Equation (3.67).

3.4.7 Simulation of a reference case for hot surface ignition

The experimental results from Smyth and Bryner [1] are used to validate the modelling approach suggested above. Smyth and Bryner [1] conducted experiments where a premixed flow of fuel and air at 298 K exits a circular quartz chimney at 0.16 m s⁻¹ and impinges on a small rectangular (0.0206 m by 0.0200 m) heated foil surface inclined at 45° to the flow (Figure 3.8). This experimental set up gives a short contact time between the flammable mixture of fuel and air and avoids any stagnation points on the foil surface. The metal foil is electrically heated and thermocouples measured the metal foil surface temperature. The experiment is conducted in an open loop, with an exhaust hood drawing away unburnt gas and combustion products. The foil temperature is increased at a rate of 0.5 K per second until the onset of ignition. Once ignition occurs, the foil temperature is lowered and the process is repeated 5 times for each set of parameters. Ignition is defined as the onset of visible

flames and from the thermocouple readings. Three different metal foils and several fuels are tested, including methane gas.

Figure 3.8. Foil and inlet in Smyth and Bryner's [1] experimental setup

3.4.7.1 Simulation setup

The simulation domain used in the present study is the region of space enclosed by the dots, the foil surface and the inlet in Figure 3.8 and located on the foil centerline. For efficient workflow, the simulation domain is a thin slab 0.002 m thick while the mesh near the foil is highly refined. The details of the boundary conditions applied are listed in Table 3.5 and their locations shown in Figure 3.9. Periodic boundaries are applied to both sides of the slab-shaped domain. For the temperature field, the “Upper Fold” and “Lower Fold” surface uses an adiabatic boundary condition as the actual temperature is uncertain but clearly lower than the temperature of the “Heated Foil” surface. An adiabatic boundary condition adds or takes away no energy from the flow field, especially for the gas mixture just leaving the “Heated Foil” surface and going above the “Upper Fold” surface. This retains more energy in the flow field surrounding the

foil, increasing reactivity, leading to an underestimation of the temperature of the “Heated Foil” surface that supports ignition. This is aligned with the underestimations that other implementation details cause. The inlet mass fractions follow Table 3.2. The initial mass fractions are $Y_{Ar}=0.014065$ and $Y_{O_2}=0.234510$. Nitrogen is the constraint material. The mass fraction of other mixture components not listed is zero.

The $k-\omega$ Shear Stress Transport (SST) turbulence model and a mesh with suitably thin first layer thickness ($y^+ \leq 1$) is used for accurate boundary layer modelling. While the low flow speed over the plate seems to allow a laminar flow simulation, the flow field becomes turbulent as pockets of hot product gases separate the inlet flow from the plate. For greater generality, turbulent intensity of 0.050, which is also a default value in the software, is introduced into the domain via the inlet flow.

Table 3.5. Boundary conditions applied in the numerical implementation of the Smyth and Bryner [1] experiment

Surface name	Boundary type	Mass & Momentum	Energy	Turbulence	Mixture components
Inlet	Inlet	$u = 0.00 \text{ m s}^{-1}$ $v = 0.16 \text{ m s}^{-1}$ $w = 0.00 \text{ m s}^{-1}$	Inlet temperature 295.0 K	Turbulence intensity 5%	Inlet mass fractions for Ar, O ₂ & CH ₄ .
Heated Foil	Wall	Smooth Non-slip	Test temperature	-	-
Upper Fold Lower Fold	Wall	Smooth Non-slip	Adiabatic	-	-
Air Wall 0 to Air Wall 5	Opening	Entrainment with Zero Pressure difference	Far field Temperature 295.0 K	Zero gradient	Far Field mass fractions for Ar & O ₂ .

Transient simulations are used for simulating the effects of finite rate chemistry. From implementing the selected reaction mechanism for a pocket of gas fully enclosed in a box with no heat loss, the largest time step that gives outcomes

independent of time step for a fully adiabatic progression of the reaction is 1.0×10^{-8} s. Since there is heat lost in the simulation domain, the reaction is slightly less vigorous and time steps such as 1.0×10^{-6} s or 1.0×10^{-7} s are used.

Figure 3.9. Computational domain encompassing the foil

3.4.7.2 Mesh setup and refinement

Due to the 45° angle of the heated foil and the small gap between the lower edge and the inlet, a fully structured mesh is not possible. Tetrahedral cells are used for unstructured meshing as seen in Figure 3.10 to Figure 3.12. The cell size on the heated foil surface is at most 5.0×10^{-5} m, guided by the simulation setup of Saiki et al. [111]. The heated foil surface details for the 3 meshes used in the present study are summarised in Table 3.6.

Table 3.6. Mesh details of domain in the present study

Mesh Name	Number of nodes	Cell size on heated foil surface	Approximate 1 st layer thickness
Fitted	295912	5.0×10^{-5} m	4.375×10^{-5} m
FittedRefine01	421728	5.0×10^{-5} m	0.822×10^{-5} m
FittedRefine02	510509	4.0×10^{-5} m	0.616×10^{-5} m

When the reaction progresses from ignition to the end of the rapid temperature rise phase with parameter set “VIGR2”, the coarsest mesh “Fitted” returns $y^+ \leq 0.5$ for the heated foil surface at 1380.0 K, 1390.0 K and 1400.0 K.

Figure 3.10. Mesh surrounding the foil along the foil centerline

Figure 3.11. Mesh surrounding the foil along the foil centerline – first refinement

Figure 3.12. Mesh surrounding the foil along the foil centerline – 2nd refinement

The larger cells away from the foil prevents the overall residue values for the mass and momentum equations from reducing below 1.0×10^{-4} . The grid convergence index by Celik [112] is not computed but the transient variation of CO_2 mass fraction in Figure 3.14 at point B (indicated in Figure 3.13) shows that the 2 refined meshes are sufficient for obtaining consistent outcomes near the foil surface since the CO_2 mass fraction vs. time plots are qualitatively similar.

Figure 3.13. Location of perpendicular lines and monitor point B

Due to the large refinement from mesh “Fitted” to mesh “FittedRefine01” (42% increase in nodes), the time step used is reduced to 1.0×10^{-7} s all meshes to ensure that the Courant number is the same or reduces.

(A) The foil at 1380 K

(B) The foil at 1390 K

(C) The foil at 1400 K

Figure 3.14. Carbon dioxide mass fraction at point B after mesh refinement

3.4.7.3 Ignition temperature independent of material

Ignition temperature for flowing methane-air mixtures is demonstrated clearly to be a function of surface material and equivalence ratio in the experiment

outcomes of Smyth and Bryner [1]. The temperatures that ignited the flowing mixture of methane and air at equivalence ratio of 0.7 is 1252 K for stainless steel, 1332 K for the titanium foil and 1367K for the nickel foil surface and this range widen as equivalence ratio increases, as shown in Figure 1.2.

To model the common lean mixtures generated by natural gas leaks, the present study models the experiment using flowing methane-air mixtures at equivalence ratio 0.7. The Smyth and Bryner [1] experimental outcomes indicate that the spread of ignition temperatures very likely narrows below equivalence ratio 0.7. Therefore, the influence of material is considered to diminish towards lower lean equivalence ratios, consequently only the chemistry model for the gas phase is implemented.

Since the ignition temperatures across the 3 materials are in a narrow range of 115 K compared, which is acceptably small compared to the mean ignition temperature 1317 K, it would be reasonable to argue that temperature is the main driver of ignition. Modelling only the gas phase chemistry does bring a sense of generality to this approach, which is useful especially when a heated surface is of unknown material.

The material of the surface would also affect the identified hot surface ignition temperature by heat conduction away from the surface and quenching of radicals on the surface. However, in the present study, the Van't Hoff ignition criterion on the foil surface prevents defining a heat flux on the foil surface and

the 2-step ignition model does not contain radicals, leaving temperature at the surface as the only driver for hot surface ignition.

3.4.7.4 Implementing the Van't Hoff ignition criterion

The ignition criterion is the Van't Hoff criterion described in Laurendeau [85]. The temperature of the gas mixture is recorded along 9 regularly spaced lines normal to the foil surface as shown in Figure 3.13. The heated foil transfers thermal energy to the mixture of methane and air as it travels up the foil surface. With the foil at 1400 K and as the reaction progresses (using "VIGR2" Arrhenius parameters), the gas mixture at line 9 demonstrate the change in temperature gradient that indicates ignition according the Van't Hoff ignition criterion. The temperature gradient at line 9 changes from negative (time 0.000475 s) to zero to positive (time 0.000575 s) in Figure 3.15 as heat production by the reaction begins to exceed heat transfer from the wall to the fluid.

The visualization of the Van't Hoff criterion on the wall at the identified ignition temperature is possible without a fine mesh on the wall. A fine mesh results in sufficient spatial resolution near the wall so that at least a few cells can hold the same temperature information at the wall, otherwise the zero temperature gradient is found only across a single cell and the predicted result is lost in the visualization.

Figure 3.15. Change in temperature gradient indicating ignition (Van't Hoff criterion)

3.4.8 Identifying the hot surface ignition temperature

Transient turbulent simulations are carried out to reproduce the ignition temperature of Smyth and Bryner [1] for methane gas. The foil temperature rises 0.5 K per second and when interpreting this as a mean rate, it becomes possible to consider the heated foil surface spending 2 seconds at each temperature (to the nearest Kelvin) as illustrated in Figure 3.16.

Figure 3.16. Staying at each temperature for 2 seconds

3.4.8.1 Preparing the Initial values

For each temperature tested, the flow, temperature, and chemical species fields are prepared this way before the start of these 2-second intervals. Steady-state simulations determine the flow field and temperature field. The test temperature is the temperature of the foil. Reactions are disabled and the chemical species are distributed over the domain by the flow field and temperature field. Once the flow, temperature and chemical species distributions show very little change, this steady-state result forms the initial value file of the transient simulation. When the transient simulations begin, chemical reactions are enabled. Since reactions are disabled, there accumulates a pocket of methane gas heated by the foil but not reacting, which is unphysical. Since the ignition temperature is identified by this approach, the assumption is that the temperature below the current tested temperature is too low to cause ignition and the domain is still filled with unreacted methane. The CH_4 mass fraction on the foil leading up to ignition with the foil at 1400 K shows small differences (Figure 3.17), implying that if the foil is at a lower temperature before reaching 1400 K, that would not have altered the distribution of CH_4 . This difference is small because the “VIGR2” Arrhenius parameters for reaction step 1 have high activation energy.

Figure 3.17. The methane mass fraction on the foil at the time of ignition with the foil at 1400 K

Chapter 4. RESULTS

The Results chapter presents the outcomes of un-stacking the LM2500 axial compressor. To assess the validity the information from the un-stacked LM2500 axial compressor, a set of stage flow angles is used to construct a heavily simplified flow path found running between 2 adjacent blades at blade row in each stage and through all stages and the flow field set up within this geometry is assessed via computational fluid dynamics. Concurrently, the 2-step reaction mechanism for methane combustion embedded in the numerical implementation of the hot surface experiment is tested with the hot surface at temperatures separated by 10 K steps between 1300 K and 1400 K to identify the temperature that causes ignition. Lastly, the sequence of events occurring on the heated surface, including ignition and rapid temperature rise is examined in more detail.

4.1 Stage un-stacking method an axial compressor

A basic axial compressor from the Section “Building a basic axial compressor” is “designed” with the following considerations to study the influence of the IGV flow turning angle, the OGV inlet angle, the pressure ratio models and the SLC models. The SLC is constant for the non-VGV stages and also constant SLC for the VGV stages (SLC model 1). The distribution of stage pressure ratios is based on fully isentropic compression using specific entropy as a function of temperature and pressure applied to each stage (Pressure ratio model 3). The blockage from boundary layer shedding off the blades as wakes and stationary wall boundary layers is set to grow to a maximum of 10% of the cross sectional

area, supported by Pedersen [6]. The “design” goal is to reduce the mean amount of mismatch in flow angles at the stator-outlet-rotor-inlet interfaces. The simplified solution procedure, where, the specific stage stagnation enthalpy rise is assumed similar to the specific stage static enthalpy rise, $\Delta h_{\text{TOT.STG}} \approx \Delta h_{\text{STG}}$ is used to remove the need to iterate, sacrificing improved results for design turn-over speed. Using the stage un-stacking method, a large collection of data is generated for a range of IGV flow turning angles and OGV inlet flow angles (before the OGV straightens the flow), to locate the design space where the mismatch in flow angles is zero for the axial compressor’s design operating point.

4.1.1 Effect of increasing IGV flow turning angle

Applying the stage un-stacking method to study the effect of increasing the IGV flow turning angle, Figure 4.1 shows the data generated for IGV flow turning angles from 20° to 34° and for selected rotational components of the absolute velocity at the OGV inlet. The rotational component v is a fraction, varying from 0.42 to 0.52, of the OGV inlet wheel speed, defined in the same form as in Equation (3.23). Each data point represents a set of design choices that results in a feasible set of flow angles for the whole compressor.

Figure 4.1. The effect of flow turning angle in the IGV at various OGV inlet angles which are specified by fraction of wheel speed

As both the IGV flow turning angle and v , the fraction of wheel speed, increase towards the optimum combination of IGV flow turning angle of about 31° and v close to 0.46 of the OGV inlet wheel speed, it becomes possible to obtain a set of feasible flow angles for the axial compressor as a whole that achieves minimal mismatch in flow angles at each stator-outlet-rotor-inlet interface between stages. However, as the fraction of wheel speed increases further, it again becomes increasingly difficult to obtain a set of feasible flow angles for the whole compressor. Since the axial compressor's design is highly optimized,

the many design parameters simultaneously match narrowly about the design point.

4.1.2 Effect of OGV inlet flow angles

The velocity components u and v at the OGV inlet determines the outlet flow angle at the last stage's stator. An improved estimate of the specific stagnation enthalpy at the OGV inlet requires the rotational component v before allocating sufficient specific static and stagnation enthalpy to each axial compressor stage. Using the same generated data for IGV flow turning angle, the effect of OGV inlet flow angle is examined by varying v and presented in Figure 4.2. Each data point in Figure 4.2 represents a set of design choices that results in feasible set of flow angles across the whole compressor. For clarity, only the even IGV flow angles are shown.

Figure 4.2. Increasing the fraction of wheel speed at the OGV inlet

Increasing v as a fraction of wheel speed at the outlet has only a small effect on reducing the amount of mismatch in flow angles at the stator-outlet-rotor-inlet interface. Adjustments to v hardly minimise the flow angle mismatches unless the IGV flow turning angle is close to 31° for this axial compressor.

4.1.3 Effect of pressure ratio model

The effects of different pressure ratio models on an axial compressor's flow angles at the design point are examined with a basic compressor, where the IGV flow turning angle is 28° and at the OGV inlet, $v = 0.45$ of the wheel speed. The SLC model 1 is used to set the axial temperature distribution, relying on the assumption $\Delta h_{\text{TOT.STG}} \approx \Delta h_{\text{STG}}$. The combined effect of the choice of pressure ratio model and the method that smooths the velocity distribution has minimal effect on the mean flow angle mismatch at the stator-outlet-rotor-inlet interfaces as seen in Figure 4.3. The pressure ratio models only distribute available pressure among the stages of the axial compressor. Within the overall compression ratio of this axial compressor, any additional rise in pressure ratio in a stage is compensated with a lower pressure ratio in another stage. For example, the lower pressure ratios at the rear stages suggested by pressure ratio model 3 are complemented by higher pressure ratios in the front stages and the reverse occurs pressure ratio models 1 in Figure 4.4B.

Figure 4.3. Mean flow angle mismatch between pressure ratio models

The choice of pressure ratio model, however does affect the maximum pressure ratio available at each stage as seen in Figure 4.4A, where pressure ratio model 3 delivers more compression in the front stages compared to pressure ratio model 1 and 2. This effect is present in a small way in the actual stage pressure

ratios in Figure 4.4B. The estimated stage pressure ratio is closer to the actual from only stage 5 onwards. The “PR GE LM2500” data in Figure 4.4B is taken from Klapproth et al. [71].

(A) Maximum available stage pressure ratio

(B) Actual stage pressure ratio

Figure 4.4. Maximum and used Pressure ratios across whole compressor when different pressure ratio models are used

The resulting axial velocity profile in Figure 4.5 is smooth at the front stages even after factoring the effect of blockage. However, when moving from the last VGV stage to first non-VGV stage, there is a rougher transition. This would happen as this stage un-stacking method has no provision for transiting the flow from a VGV stage to a non-VGV stage. For the same mass flow rate, the axial velocity distribution from pressure ratio model 3 in Figure 4.5 do indicate lower axial velocities, implying higher density from higher pressure ratios in the front stages.

Figure 4.5. Stage axial velocity with different pressure ratio models

Considering that the actual axial velocity distribution (“Act. Ax. Vel.” in Figure 4.5) from Klapproth et al. [71] is not always smooth, the rough transition in axial velocity is accepted. According to the approximate compressor schematic on the gas turbine manufacturer’s marketing datasheet [92], there is a proportionally longer stator at stage 8. The 8th stage stator houses the bleed air valve, according to Klapproth et al. [71]. In the non-VGV stages, the axial speeds show the greatest difference. This difference is traced to several possible sources, the OGV, bleed air, annulus cross sectional area and blockage.

The OGV is mentioned by Klapproth et al. [71] but there is too little information on the cross sectional area and the axial length for a proper analysis of the flow speed. Should the OGV be part of the analysis, it would also contribute to pressure rise. The OGV will reduce the stage loading of all stages as some pressure and temperature rise is obtained through straightening the flow. This would mildly but clearly reduce stage compression, leading to lower stage density at the last stages. To maintain the same mass flow rate, the axial speeds must increase. Therefore, the OGV excluded from the analysis is not a

cause of higher axial flow speed at the last stages. In addition, inferring the radius from the same approximate compressor schematic on the gas turbine manufacturer's marketing datasheet [92], there is little change in cross sectional area after the last compressor stage, implying axial mass flux might keep constant after flow straightening. Since pressure increases to give higher density through the OGV, lower axial speed results after the OGV to maintain mass flow rate. This would not affect the axial speeds of the last compressor stages. Bleed air for film cooling in the high pressure turbine is interpreted as obtained from the compressor discharge according to the technical section of this 3rd party market analysis [8], and does not affect the axial speed at the last stages. Similar no-blockage annulus cross sectional area is found by estimating the radius from the same approximate compressor schematic on the manufacturer's marketing datasheet [92] and using data in Pedersen [15]. The estimated radius from the same approximate compressor schematic on the manufacturer's marketing datasheet [92] results in a slightly larger annulus cross sectional area. The Blockage model supported by data in Pedersen [6] shows a clear 10% reduction in available cross sectional area after stage 9 as indicated in Figure 3.6. This level of blockage is used at the OGV inlet. To resolve this obvious difference in axial speed in the 2nd half of the compressor especially at the OGV inlet, certain modeling improvements are possible. The extraction of bleed air for turbine cooling must be considered and a better estimated annulus cross sectional area is needed. As the analysis is at the design operating point and approximate, the further information on the VGV operation from Klapproth et al. [71] for this gas turbine is not used.

For the same SLC model, the rotor blade row needs to deliver a similar specific stage stagnation enthalpy rise in all 3 pressure ratio models. When pressure ratio model 3 delivers lower stage axial velocity (Figure 4.5) compared to the other pressure ratio models, the rotor needs to turn the flow by a greater angle to deliver a larger rotational component of the absolute velocity that compensates for the reduced axial component of the absolute velocity, according to the Euler whirl equation. This leads to pressure ratio model 3 generating slightly larger rotor blade angles compared to the other pressure ratio models in Figure 4.6A. Consequently, since the rotor blade row is delivering a larger rotational component of absolute velocity with pressure ratio model 3, and the stator blade row need only conserve specific stagnation enthalpy, the inlet and outlet velocity triangles of the stator blade row are more similar. Consequently, the stator blade angles are slightly smaller compared to that obtained in the other pressure ratio models in Figure 4.6B.

(A) Rotor blade camber angle and zoom in

(B) Stator blade camber angle and zoom in

Figure 4.6. Blade camber angles with different pressure ratio models

In the actual compressor, by the same argument, the much lower axial speed will result in larger blade cambers, resulting in differences between the blade cambers obtained in this stage un-stacking method and the actual (“Tip Camber” and “Hub Camber” in Figure 4.6).

By deliberate design in this stage un-stacking method, the β_1 angle is consistent or allowed to vary only slightly across the stages. Since the β_1 angle could keep constant in Figure 4.7A with only slight variations at the first 3 stages to accommodate determining the other flow angles, this assumed β_1 design guide is feasible. Assuming that the effects of the RSRR initial design persist after many design iterations, the stage α_2 angle would also likely be as consistent as

stage β_1 angle. Without constraining the stage α_2 angle, this stage un-stacking method has determined a distribution of α_2 angles that is relatively consistent, if not smoothly varying, especially for the non-VGV stages (Figure 4.7B). It is possible that the studied axial compressor maintains signs of the RSRR initial design, especially at the non-VGV stages. The angles, α_2 and β_1 from stage un-stacking are much closer to the actual than the blade camber angles in Figure 4.6. Should lower axial speed be used at the last stage, the last stage β_1 angle would be larger. Since this stage un-stacking method has the capability to slightly reduce the β_1 angle as the analysis proceeds towards the front of the compressor, it would be possible that beginning with a larger β_1 angle the last stage, this stage un-stacking method is able to estimate a β_1 angle distribution closer to the actual.

(A) Stage β_1 flow angle

(B) Stage α_2 flow blade angle

Figure 4.7. Flow angles with different pressure ratio models

4.1.4 Effect of SLC distribution

The effects of different SLC models on an axial compressor's flow angles at the design point are examined with the same basic compressor, except that pressure ratio model 1 is used and the SLC model varies. The IGV flow turning angle is still 28° and at the OGV inlet, $v = 0.45$ of the wheel speed.

Compared to the different pressure ratio models, the choice of SLC model has a larger effect on mean flow angle mismatch at the stator-outlet-rotor-inlet interfaces than for the choice of pressure model as seen in Figure 4.8. Using these design options, the SLC model 3 where there is a constant specific static enthalpy rise for all stages could not support generating a complete feasible set of flow angles that fit all stages. While generating the velocity triangles from the OGV inlet to the compressor's 1st stage with SLC model 3, the available energy and requirements could not set up a proper velocity triangle at a middle stage within this axial compressor.

Figure 4.8. Comparison of mean flow angle mismatch between SLC models

The stage SLC distribution in Figure 4.9 shows that SLC model 3 with constant specific stage static enthalpy rise has the lowest SLCs for the non-VGV stages. The compressor designed with SLC model 3 imparts lesser specific stagnation enthalpy to the working fluid when higher rotational kinetic energy (ωr_E) is available at the rear stages. At the same time, the front stages must impart higher specific stagnation enthalpy to the working fluid when lesser rotational kinetic is available as the Eulerian radius, r_E is smaller. This mismatch is the

reason SLC Model 3 could not set up a proper velocity triangle at one of the middle stage within this axial compressor.

Figure 4.9. Stage SLC distribution with different SLC models

The specific stage static enthalpy rise in Figure 4.10 reveals the same trend as stage SLC since the simplifying assumption that $\Delta h_{TOT.STG} \approx \Delta h_{STG}$ is used in the SLC definition. Because SLC model 3 could not support in finding a complete set of flow angles for the whole axial compressor, the specific stage static enthalpy distributions in SLC models 1, 2 and 4 indicate that specific stage static enthalpy rise must increase stage after stage for this axial compressor. The specific stage static enthalpy-rise in model 2 is not a smooth curve as the temperature-specific static enthalpy function is only sufficiently piecewise smooth.

Figure 4.10. Specific stage static enthalpy rise with different SLC models

In this stage un-stacking method, the stage pressure ratios cannot be fixed while varying the stage load coefficient because only the variation in pressure ratios is available for smoothing the axial velocity especially from the IGV to the 2nd stage of the axial compressor. However, the difference in stage pressure ratios in Figure 4.11 are small from stage 5 onwards. The major difference is found in stages 1 to 4, where higher specific static enthalpy rises (Figure 4.10) corresponds to higher pressure ratios (Figure 4.11).

Since the compressor inlet axial speed is known, each SLC model works with the same pressure ratio model to generate the same inlet density, resulting in pressure and temperature moving in tandem at the inlet. In the subsequent stages, for the same mass flow rate and known smooth cross-sectional area variation, a smooth density variation is needed to generate a smooth axial velocity profile. This smooth density variation further maintains the differences in pressure ratio for the front few stages.

Figure 4.11. Stage pressure ratios with different SLC models

By the 2nd stage in the axial compressor, Figure 4.12 suggests that the axial velocity is no longer influenced by the conditions at the compressor inlet. In SLC model 1, due to the initial lower pressure ratios, the resulting lower density flow is compensated by increasing the axial velocity through the rest of the axial compressor. The opposite occurs for SLC model 3, which has the highest initial compression of the 4 SLC models.

Figure 4.12. Stage axial velocity with different SLC models

4.1.5 A selected set of blade angles and flow angles

To test in 3D, the feasibility of the estimated mean stage axial velocity, mean stage pressure ratios, mean specific stage static enthalpy rise, and stage flow angles obtained from the stage un-stacking method, a 1/72 slice of an

axisymmetric 3D axial compressor is simulated. From the Section “Effect of SLC distribution”, the set of flow angles determined with SLC model 1 is selected since it contains a small but acceptable average absolute difference in flow angles at each stage-outlet-stage-inlet station. These inputs (IGV flow turning angle is 28° and $v = 0.45$ of the wheel speed at the OGV inlet) are used to determine a possible set of angles at the design operating point but since no further optimisation takes place, there exists a small angle mismatch at the stage-outlet-stage-inlet interfaces. The 16 sets of blade angles, combined with the estimated stage axial lengths are used to estimate the circular arc camber lines of the rotor and stator blades.

When the simplifying assumption $\Delta h_{TOT.STG} \approx \Delta h_{STG}$ is removed, the same set of inputs (IGV flow turning angle is 28° and $v = 0.45$ of the wheel speed at the OGV inlet) does not give a converged set of angles for the whole compressor. Since IGV inlet turn angle exerts a major influence, it is adjusted while keeping the other factors the same. Without assuming $\Delta h_{TOT.STG} \approx \Delta h_{STG}$, the smallest IGV flow turning angle found is instead 32.7° , while searching by 0.1° increments. Meanwhile, the magnitude of the mean angle mismatch per stage has decreased from 0.206° to 0.123° . After obtaining converged specific stage stagnation enthalpy rise at each stage, this ratio $|\Delta h_{TOT.STG} - \Delta h_{STG}|/\Delta h_{TOT.STG}$ is usually $\pm 1\%$ at most stages, with a maximum of 4% at one of the front stages. Therefore, generally the small differences due to the simplifying assumption, $\Delta h_{TOT.STG} \approx \Delta h_{STG}$ are acceptable, conferring the benefit of faster calculation. The 3D checking proceeds with velocity, pressure, enthalpy and angles obtained using the assumption $\Delta h_{TOT.STG} \approx \Delta h_{STG}$.

The workflow for models and information used during checking the SUSM outputs with CFD simulation is shown in Figure 4.13. The stage un-stacking method (SUSM) and CFD simulation use the same mass flow rate, stage cross sectional areas and high-pressure spool RPM, among other variables.

Figure 4.13. Workflow for models and information used during checking the SUSM outputs with CFD simulation

For efficient testing, the geometrical model is simplified in the following ways. Each blade row is designed with 72 blades. The blades are only thin sheets represented by their camber lines with no thickness and no radial blade twist from the hub to casing. The gaps between each blade row are about 25% of the axial length of the blade row. The simulation domain shown in Figure 4.14 is the flow path between adjacent blades and all blade rows are aligned such that the stage inlets and outlets match. The VGV rotor blade rows are indicated in blue, while the non VGV rotor blade rows are indicated in cyan. The stators blade rows are indicated in yellow. The IGV and OGV are indicated in grey. This geometry used in CFD is designed to give only one major drawback: The lack of a convergent-divergent passage between adjacent blades. Flow diffusion will not take place, the CFD simulation outcomes should report poorer temperature and pressure rise. The smaller stage temperature and stage pressure rise will impact axial velocity.

(A) The IGV and stages 1 to 8 (B) Stages 9 to 16 and the OGV
Figure 4.14. An approximate 3D flow path between adjacent blades

The other minor drawbacks are no incidence angles at the leading edge, no flow deviation at the trailing edge, the incorrect number of blades compared to the actual and the absence of blade twist. Blade incidence angles and deviation angles are small and their absence means the blades turns the flow through a slightly smaller angle. The incorrect number of blades implies incorrect solidity. Since solidity is a design variable that seems to accept a large range of values, as demonstrated in the RSRR 1D design approach by Mattingly [60], this simplified compressor has been “designed” with a different solidity. With less solidity, the flow turns a smaller angle through the blade row. No blade twist causes inefficient flow at the casing and hub because the change in wheel speed in the velocity triangle is ignored. Due to the short blade spans, this difference is manageable. The flow becomes inefficient and does not separate.

The simulation software is ANSYS CFX versions 18.0 and 18.1, used with a research license. This allows the mesh to reach 9.5 million nodes. The blade surfaces hub surface and casing surface are walls of specified temperature. The gaps between blade rows have periodic walls. The mesh is structured and concentrated towards the blade surfaces, the periodic walls and the interfaces

between stages. The interface between blade rows is the plane equidistant from the previous blade's trailing edge and the following blade's leading edge. The IGV, stators and OGV form the stationary domain while only the rotors form the rotating domain. The rotating domain is set to the design RPM, which is the RPM of the operating point with the largest power output. The "General Connection" model is used at the domain interfaces with "Frozen Rotor" as the "frame change option". The "Conservative Interface Flux" is used for mass and momentum conservation, with the mass flow rate maintained by adjusting pressure through a "Pressure Update Multiplier". The turbulence model is Shear Stress Transport with 10% turbulence intensity at initialization and at the inlet. A higher turbulence level is selected to represent the wakes from an upstream stator blade row sliced by the downstream rotor blade row.

The same simulation is carried out on 4 different meshes with 1.2 million, 2.4 million, 4.7 million and 9.5 million nodes. The variables critical to the study are temperature, pressure and axial velocity in the free stream and at the walls. Since the mesh heavily concentrates much more cells at the walls, area averages of the temperature, pressure and axial velocity are obtained from a curved plane located at 1% of the annulus gap away from the casing wall in the stage 4 rotor blade row. This plane is just outside of or immersed in the boundary layer on the casing. The single stand-alone arrow in Figure 4.14A indicates the stage 4 rotor casing wall. Using the method and error types outlined by Celik et al. [112] to analyse the mesh refinement for the 3 finest meshes, the errors are listed in Table 4.1.

Table 4.1. Mesh refinement errors when simulating the flow in an approximate 3D flow path between adjacent blades

Variable	Apparent order	Approximate error	Extrapolation error	GCI (fine)
Temperature	0.7153	0.7942%	4.1687%	5.4376%
Pressure	8.7884	0.2659%	0.0388%	0.0485%
Axial velocity	16.071	0.9502%	0.0225%	0.0281%

The mesh with 9.5 million nodes gives y^+ values ranging about 10 to 20 on the blade surfaces. The highest y^+ is 115 on a few pockets on the casing towards the OGV. On the casing, the y^+ is mostly about 60 to 70, while on the hub, the y^+ is about 40 to 50. However, as most of the errors in Table 4.1 are below 1%, following presented simulation outcomes are obtained from the mesh with 1.2 million nodes. This coarser mesh gives y^+ values from 0 to 4100, distributed in a similar way. Between the finer mesh and coarser mesh, the velocity vectors are behaving similarly.

The mean stage outlet temperatures from CFD achieve about a third of their intended temperature rise compared to that obtain in the stage un-stacking method (legend details: SUSM) as shown in Figure 4.15A. The axial profile of the minimum, mean and maximum temperature from CFD are however, qualitatively similar to the SUSM temperature profile (Figure 4.15A), implying that the 3D calculations of temperature in the axial compressor are working towards the stage un-stacking method outcomes. The spread of temperatures at each stage shown in Figure 4.15B, though not small, stabilizes at the non-VGV stages. This indicates that the 3D calculations are also converging towards a stable spread in temperatures. The temperatures are obtained from the stationary side of each interface.

(A) Axial temperature profile

(B) Percentage difference of mean at each stage outlet

Figure 4.15. Axial temperature for stage un-stacking method and CFD

The distribution of temperatures at the stage 4 and stage 12 outlets is shown in Figure 4.16A. The stage 12 outlet shows clearly that the higher temperatures are concentrated at the casing wall. The anticipated stage temperature rise applied on the casing wall as a Dirichlet temperature boundary condition is higher than the temperature rise this compressor is able to deliver.

The reason for the lower temperature rise is traced to the absence of blade thickness leaves the existing thin walls to provide only a mildly converging and diverging flow passage, which does not sufficiently flow accelerate and decelerate the flow, and does not give the accompanying static temperature rise. This causes each stage to fulfill less than their intended temperature rise.

(A) Temperature distribution at stage 4 and 12 outlets

(B) Pressure distribution at stage 4 and stage 12 outlets

Figure 4.16. Contours plots from CFD for temperature and pressure from CFD

The mean stage outlet pressure from CFD are in good agreement with the SUSM pressure rise, except at the last 5 to 6 stages. At front stage outlets, Figure 4.17A shows that the profile of the minimum, mean and maximum pressure obtained from CFD are close to the pressure profile used in the stage un-stacking method. The range of minimum to maximum pressure at each

stage outlet in Figure 4.17B, though not small, stabilizes at the non VGV stages mainly due to the large mean pressures. The pressures are obtained from the stationary side of each interface.

(A) Axial pressure profile (B) Percentage difference of mean at each stage outlet

Figure 4.17. Axial pressure for stage un-stacking method and CFD

The distribution of pressure at the stage 4 and stage 12 outlets is shown in Figure 4.16B. Both stage outlets display mild pressure variation.

A critical look at Figure 4.17A, the pressure profile from CFD does not reach the SUSM pressure profile in the last 5 to 6 stages. Especially at the last stages, shortfalls in pressure rise in the earlier stages will keep the later stages from reaching the SUSM stage pressure targets. As is the case for temperature, the reason there is gradually insufficient pressure rise, is the lack of the convergent-divergent that delivers the require static pressure rise as the flow is accelerated and decelerated.

Tracing back to the CFX software's recommended simulation approach, the inlet pressure and density field is allowed to vary so that mass flow rate is conserved. In contrast, the outlet pressure is fixed with a Dirichlet boundary

condition. Since the outlet pressure is fixed, and when each stage does not fully realize its pressure rise in this 3D simulation, the inlet pressure increases to compensate as seen in Figure 4.18, where the pressure ratio is 1.27 at the IGV inlet (stage “-1”).

(A) Pressure ratios for stage un-stacking method and CFD

(B) Axial velocity for stage un-stacking method and CFD

(IGV inlet: stage -1, IGV outlet: stage 0)

Figure 4.18. Comparing outcomes from stage un-stacking method and CFD

The axial mean velocity profile from CFD is clearly slower than that calculated from stage un-stacking while the profile is the similar. While a simple narrowing of the passage between blades in the CAD geometry may account for the mechanical blockage presented by the blades and may accelerate u_{CFD} to the intended levels, this approach was not thought of within the allocated time.. However, this alternative correction approach begins by incorporating blockage that reduces effective flow area. The stage un-stacking method and CFD simulation use the same mass flow rate, stage cross sectional areas and high-pressure spool RPM. Therefore, the following relations are used at each stage.

$$\dot{m} = (\rho Au)_{\text{SUSM}} = (\rho Au)_{\text{CFD}} \quad (4.1)$$

where u is the axial velocity. In SUSM, corrected cross sectional area is used, where there is mechanical blockage such that the remaining area is $A_{\text{SUSM}} =$

BA_{CFD} , where B represents the remaining flow area. The shed wakes cause the same amount of blockage in both approaches. This changes Equation (4.1) into

$$(\rho u)_{SUSM}BA_{CFD} = (\rho u)_{CFD}A_{CFD} \quad (4.2)$$

Removing the common variables gives

$$(\rho u)_{SUSM}B = (\rho u)_{CFD} \quad (4.3)$$

$$\frac{u_{SUSM}B}{u_{CFD}} = \frac{\rho_{CFD}}{\rho_{SUSM}} \quad (4.4)$$

Since blockage B ranges $0.9 \leq B \leq 1.0$, and $u_{SUSM}B > u_{CFD}$, ρ_{CFD} is higher than intended at all stages. In the CFD simulation, the higher stage density can only arise from lower stage temperature and not lower stage pressure. This confirms that stage temperatures are lower than intended, which agrees with the preceding observations that the stage temperature rises are less than intended. In a compressor, the energy that supports a stage temperature rise comes only from converting rotational kinetic energy of the high-pressure spool to thermal energy. The poorer energy conversion is traced to the lack of a sufficiently converging-diverging passage between adjacent blades.

This lower mean axial velocity is also due to the absence of blockage throughout axial compressor as the blades are only their camber lines, there is no blockage contributed by blade thickness, also causing lower axial velocities.

In the 3D CFD simulation, the lower axial speeds and wheel speed together produce velocity vectors that are still able to follow the blade curvature. At the blade inlet and outlet stations, the velocity triangles based on the mean velocity values from the 3D CFD simulation, being uncorrected are currently giving larger α and β angles with larger absolute and relative velocity magnitudes. The

blade curvatures remains relatively constant as the both α angles at the stator and both β angles at the rotor adjust by similar amounts. At the same time, the blade chord lines rotate through an angle similar to the change in α and β angles. However, the axial velocity needs to be corrected by increasing 27% to 60% to match that obtained by the stage un-stacking method at the design operating point. The wheel speed needs no correction. The axial velocity correction that adjusts the velocity vectors so that they follow the blade curvature more closely is derived beginning with conservation of mass flow rate and followed by a correction on effective flow area and density, as carried out above. Using the Gas law, the density in Equation (4.2) is expressed in pressure and temperature

$$\rho_{\text{SUSM}} = P_{\text{SUSM}} / (RT_{\text{SUSM}}) \quad (4.5)$$

$$\rho_{\text{CFD}} = P_{\text{CFD}} / (RT_{\text{CFD}}) \quad (4.6)$$

The density terms are replaced in Equation (4.2) to give

$$\frac{P_{\text{SUSM}}}{RT_{\text{SUSM}}} u_{\text{SUSM}} B = \frac{P_{\text{CFD}}}{RT_{\text{CFD}}} u_{\text{CFD}} \quad (4.7)$$

Since the corrected temperature and pressure must follow the values obtained in the stage un-stacking method, $T_{\text{CFD.Corr}} = T_{\text{SUSM}}$ and $P_{\text{CFD.Corr}} = P_{\text{SUSM}}$. Rearranging Equation (4.7) and incorporating the subscript changes for temperature and pressure gives Equation (4.8), which is used to correct the axial mean velocity. The CFD quantities are mean values.

$$u_{\text{CFD.Corr}} = \left(\frac{T_{\text{SUSM}}}{T_{\text{CFD}}} \right) \left(\frac{P_{\text{CFD}}}{P_{\text{SUSM}}} \right) \left(\frac{1}{B} \right) u_{\text{CFD}} \quad (4.8)$$

The velocity vector plots for the IGV, each stage and OGV of the compressor is taken at the mid-span of the blade, at 15% of the blade span from the blade root

and at 15% of the blade span from the blade tip. These plots indicate the absolute velocity field follows the flow path in the stator blade row and that none of the flow makes an about turn to give a negative axial velocity. The stage 4 and stage 12 velocity vector plots at blade mid-span are shown in Figure 4.19.

Figure 4.19. Velocity vector at stage 4 and 12 at mean line plane in stationary reference frame

In summary, 3D CFD simulation results of the LM2500 axial compressor after correction do match the results of the stage un-stacking method. Despite implementing the set of non-converged flow angle angles, the 3D CFD simulation generates a velocity field that follows the flow path and blade surfaces. This indicates that with suitable inputs, the stage un-stacking method is able to deliver a set of results, suitable for describing the individual axial compressor stages at the design operating point.

4.2 Hot surface ignition chemistry

The temperatures typically found inside a running axial compressor and the ignition temperatures of a hot metallic surface are both needed because the magnitude of the temperature difference is a form of safety factor. Should there be methane inside the axial compressor, the methane reaction must supply its

own heat to cross this temperature difference and reach the ignition temperature for the hot metallic surfaces. This temperature difference is an input to building a “safety case” for ingestion of methane into a gas turbine.

The previous section enables a highly realistic estimate of the local free stream speed over a blade surfaces within at each stage of an axial compressor. Considering the small chord of the compressor blade, usually 2 to 4 cm, the actual flow scenarios within a gas turbine may be translated into a simpler 2D-flow-over-a-flat-plate scenario. To study the effects of hot surface ignition chemistry, the present study simulates the experiment of Smyth and Bryner [1], where air mixed with methane flows over a small heated flat plate. This section presents a numerical simulation of a 2D interpretation of Smyth and Bryner [1]’s experiment for a methane-air mixture at equivalence ratio 0.7.

4.2.1 An identified Ignition temperature range

Simulations are carried out with the foil at temperatures ranging from 1200 K to 1400 K. When the foil is at 1400 K, ignition certainly takes place for both set of parameters from Table 3.3. Using the “VIGR2” Arrhenius parameters, simulation outcomes show that the time to ignition, as defined by the Van’t Hoff criterion, and the time at the end of the “rapid temperature rise” phase increases as the tested foil temperature reduces (Figure 4.20A). Simulations with the foil 1300 K reveal that this surface temperature does not support heat accumulation. The temperature rise in the gas mixture layer immediately on the wall is insufficient to reach 1300 K and the Van’t Hoff ignition criterion is not fulfilled.

No further simulations are made with the foil below 1300 K using the “VIGR2” Arrhenius parameters.

The main difference in the “VIGR2” and “MILD2” Arrhenius parameters in the step 1 reaction is that the “MILD2” Arrhenius parameters uses a lower activation energy, resulting in higher reaction rates at all temperatures from 1300 K to 1400 K (Figure 4.20B). The “MILD2” Arrhenius parameters enable ignition as low as 1200 K, but with no rapid temperature rise. The foil temperatures 1340 K, 1350 K and 1360 K are not tested as the results from lower foil temperatures indicate that ignition and rapid temperature rise are possible at these temperatures.

(A) Using the “VIGR2” Arrhenius parameters at equivalence ratio 0.7

(B) Using the “MILD2” Arrhenius parameters at equivalence ratio 0.7 (not all temperatures tested as mechanism is more reactive and still allows ignition at 1300 K)

Figure 4.20. Effect of foil temperature on time of Ignition and end of rapid temperature rise

As the foil temperature reduces, it becomes more difficult for the reaction to enter the rapid temperature rise phase. By this time, only ignition is possible and the pocket of gases on the foil surface attains the same temperature as the foil for only a short duration. The Van't Hoff ignition criterion is implemented as a monitor value with the logic in Equation (4.9) to indicate the progress of the simulations. The variable T is the local temperature at the spot on the foil where the Van't Hoff criterion is fulfilled.

$$\text{Monitor value} = \begin{cases} T, (dT/dn)_{\text{WALL}} \geq 0 \\ 0, (dT/dn)_{\text{WALL}} < 0 \end{cases} \quad (4.9)$$

The evolution of the monitor values for the Van't Hoff ignition criterion and maximum temperature are shown in Figure 4.21 for the foil at 1320 K. The Van't Hoff criterion is fulfilled for about 0.0008 s before temperatures reduce.

Figure 4.21. Monitor values for maximum temperature vs. time for the foil at 1320 K

Considering time taken to ignite and temperature rising rapidly, all “MILD2” reactions proceed quicker than the “VIGR2” reaction as seen in Figure 4.22 for the foil at 1380 K, 1390 K and 1400 K.

Figure 4.22. Effect of Arrhenius parameters on time of Ignition and end of rapid temperature rise

The ignition temperature range identified in the present study is shown in Figure 4.23 to sit well within the ignition temperatures found by Smyth and Bryner [1] for flowing mixtures. (Legend details: “SB” for Smyth and Bryner, “Temp. only” for this present study.) At equivalence ratio 0.7, the concept of an ignition temperature independent of surface material is reasonable. The 115 K spread in ignition temperatures across the 3 materials is only 8.7% of the simple mean of 1317 K.

Figure 4.23. Comparing ignition temperatures obtained in the present study to that from Robinson and Smith [16] and Smyth and Bryner [1]

The VIGR2 Arrhenius parameters together with the flow field surrounding the heated foil put an ignition temperature in the range 1300 K to 1310 K at equivalence ratio 0.7. Since the “MILD2” Arrhenius parameters enable ignition as low as 1200 K with no rapid temperature rise, this ignition temperature is below 1200 K. The reaction mechanism in the present study is for the gas phase chemistry. The surface material does not affect the “VIGR2” Arrhenius parameters. If both the VIGR2 and MILD2 Arrhenius parameters give ignition temperatures far from Smyth and Bryner [1], additional modelling of the surface chemistry will be needed to achieve a match with any of the material’s ignition temperature.

4.2.2 Ignition and rapid temperature rise driven by 1400 K surface

For the foil temperatures that lead to ignition followed by the rapid temperature rise phase, the sequence of events is examined until the time when the maximum velocity in the domain reaches 10 m s^{-1} . Beyond this speed, vortices have developed where the cells are coarse. In addition, as the mesh at the entrainment boundaries is rather coarse, an unnatural exchange of air into and out of the domain develops because the transition from air leaving the domain to air entering the domain is too abrupt and little pockets of air accelerate to supersonic speeds while entering the domain.

4.2.2.1 Ignition

The reaction proceeds fastest for the layer of methane-air mixture on the foil surface. The temperature rises and is accompanied by H_2O , CO and CO_2 gas

building up. Using the simulation where the foil temperature is 1400 K as an example, Figure 4.24 show the time before the temperature in this layer of gas mixture to reach the foil temperature before ignition occurs.

Figure 4.24. Temperature profile leading to ignition with the foil at 1400 K

Around the time of ignition, the changes in the temperature field are, however, very gradual and limited to the layer gas mixture near the foil as seen in the very similar temperature profiles on Line 9 (shown in Figure 3.13) across 5 time instances in Figure 4.25.

(A) Near the foil (B) Further from the foil
Figure 4.25. Temperature profiles along Line 9 when ignition occurs

4.2.2.2 Rapid temperature rise

After ignition, the reaction itself begins to supply sufficient amounts of energy and this, in addition to heat transferred from the foil to the gas mixture, brings the reaction into the rapid temperature rise phase (Figure 4.26).

Figure 4.26. Temperature profile leading to rapid temperature rise with the foil at 1400 K

At the end of the rapid temperature rise phase, at the site of the ignition, methane is fully consumed and in its place carbon dioxide (Figure 4.27).

(A) CH_4 mass fraction at 0.0001425 s

(B) CO_2 mass fractions at 0.0001425 s

Figure 4.27. Methane and carbon dioxide distributions after the rapid temperature rise with the foil at 1400 K

4.2.2.3 Declining temperature

After the peak of rapid temperature rise, the product gases build up gradually and cover the foil, beginning from the top of the foil. This prevents the incoming methane and air from getting into contact with the foil. The maximum temperature in the domain actually falls as seen in Figure 4.28.

Figure 4.28. Temperature profile declining after the rapid temperature rise with the foil at 1400 K

Near the end of the decline in temperature, the carbon dioxide gas has built up until it covers about three-quarters of the foil surface (Figure 4.29B). At the same time, methane gas has been consumed and is not replaced by the incoming flow (Figure 4.29A).

(A) CH_4 mass fraction at 0.004325 s (B) CO_2 mass fractions at 0.004325 s
Figure 4.29. Methane and carbon dioxide after the rapid temperature rise with the foil at 1400 K

By this time, a large pocket of gas has built up on the foil, which will leave the foil surface. The flow field is no longer aligned to the foil surface and vortices are beginning to form as seen in Figure 4.30. After this point, the velocity field becomes turbulent.

(A) During ignition at 0.000525 s (B) Large pocket of gas at 0.004325 s
Figure 4.30. Velocity vectors begin their misalignment after 0.004325 s with the foil at 1400 K

4.2.2.4 Flow field becomes turbulent

The turbulence in the flow field may be seen in the time plots for net reaction rate for the $CO - CO_2$ equilibrium (Figure 4.31) and velocity u (Figure 4.32) recorded at point B (location indicated in Figure 3.13) near the foil surface. The velocity u vs. time plot shows the flow on the foil surface switching directions. A simple Fourier analysis indicates that these oscillations are likely working in tandem at between 15000 Hz to 20000 Hz. Transient outcomes are recorded at 0.000025 s intervals, enabling analysis up to 20000 Hz. This Fourier analysis used 64 records.

(A) Oscillation in reaction rate

(B) Fourier analysis of reaction rate

Figure 4.31. Net reaction rate for the carbon monoxide to carbon dioxide equilibrium near the foil surface

(C) Oscillation in velocity u

(D) Fourier analysis of velocity u

Figure 4.32. Velocity oscillations near the foil surface

While the whole velocity field has turned more turbulent, the remaining methane is consumed (Figure 4.33) to maintain the high temperature in the flow field and on the foil surface. However, the fresh methane is prevented from reaching the foil.

Figure 4.33. Temperature profile as flow field turns turbulent with the foil at 1400 K

With no replenishments, the temperature eventually falls off (Figure 4.34).

Figure 4.34. Temperature profile as flow field prevents methane replenishment with the foil at 1400 K

Some pockets of velocities in the domain are now beyond 10 m s^{-1} and no further analysis is carried out for the reasons stated above.

Chapter 5. DISCUSSIONS

The Discussion chapter presents insights from un-stacking an axial compressor into individual stages, followed by insights from modelling hot surface ignition on heated surface. Using realistic temperature and flow speed estimates for the environment within an axial compressor, a qualitative argument is put forward to explain the possibility of hot surface ignition.

5.1 IGV flow turning angle

Using the stage un-stacking method (Sections 4.1.1 and 4.1.2), a design space is identified where the mean flow angle mismatches between the stages is close to zero. The most influential design option for reducing angle mismatches to zero is the IGV flow turning angle.

In terms of reducing the mean mismatches in flow angles per stage, varying the OGV inlet flow angle by varying v as a fraction of wheel speed at the OGV inlet exerts little influence. The mismatches stay constant and do not move to zero as seen in Figure 4.2. In applying the stage un-stacking method to this compressor, increasing v causes no increase in OGV inlet specific stagnation enthalpy since the compressor's outlet stagnation temperature is fixed. However, increasing v reduces the specific static enthalpy only slightly as the velocity contribution to specific stagnation enthalpy is small. The 10% increase in v from 42% to 52% of wheel speed at the OGV inlet results in only about 0.05 kJ/kg change in specific stagnation enthalpy at the stage before the OGV inlet. Furthermore, beyond this small 10% range of v , there are either no feasible sets

of flow angles for the whole compressor or the flow angle mismatch cannot reach zero.

In contrast, adjusting the IGV flow turning angle exerts a greater influence on reducing the mean mismatches in flow angles per stage. For solutions surrounding the optimum IGV flow turning angle that results in zero flow angle mismatches across all stages, a 1° increase in IGV flow turning angle causes a $0.2\text{--}0.5 \text{ kJ kg}^{-1}$ static enthalpy drop at the IGV outlet. For a more quantitative comparison, a 3° change about the optimum IGV flow turning angle of about 31° ($\approx 10\%$ change) causes about $0.6\text{--}1.5 \text{ kJ kg}^{-1}$ change in specific stagnation enthalpy, at the IGV outlet (stage 1 inlet), which is easily 10 times greater than the specific static enthalpy changes implemented at the OGV inlet.

Determining matching flow angles between stages and for the Euler whirl to match the specific stagnation enthalpy rise at each stage for all 16 stages of this compressor is akin to simultaneously satisfying 32 sets of requirements. These requirements and the compressor's overall pressure and temperature ratios are therefore actually coupled together to characterize the design of the studied axial compressor. This large number of constraints consequently narrows the solution range of both the IGV flow turning angle to near 31° and v to about 0.46 of the OGV inlet wheel speed for this axial compressor. However, as v at the OGV inlet has much lesser influence on flow angle mismatches than the IGV flow turning angle, the angle mismatches are efficiently first reduced by adjusting the IGV flow turning angle and if needed, followed by fine tuning with v at the OGV inlet.

5.2 Pressure ratio distribution

For the LM2500 axial compressor, shape of the pressure ratio curves obtained by applying the stage un-stacking method and the actual are only qualitatively similar (Figure 4.4B) as a stage with peak pressure ratio occurs towards the front stages. However, the stage where the peak pressure ratio occurs distinctively differs.

These 3 designs in Figure 2.4 show that aggressive pressure ratios in the early stages are more feasible than in the later stages. The important detail is which stage then delivers the highest pressure ratio. The absolute pressure rise of the first stage in the EEE would be smaller than that of the other two compressors, since the EEE design operates primarily in a low ambient pressure environment of 22631 Pa at 11 km altitude according to Frei's [113] online atmospheric pressure calculator. However, more pressure ratio distributions from actual compressors are needed before a firm design guideline may be constructed.

5.3 Acceptable range for camber angles

Noting that incidence angles and deviation angle are usually small at the design operating point, the estimated blade angles from the stage un-stacking method are well within the range 7° to 30° found in a worked example in Mattingly [60]. The RSRR approach is applied to stage stack an axial compressor, generating a large database of possible values for the design variables. The difference between the inlet and outlet flow angles of a blade row ranged from 7° to 30° .

For a NACA 65, $\alpha=1.0$ series airfoil, this translates to a camber of 1.53 to 6.58 % of the chord where the camber lines are circular arcs.

While solving for the stage flow angles, a stage with a relatively higher stage axial velocity makes for less, therefore easier, rotational velocity contributions to specific stagnation enthalpy, which in turns requires less flow turning in the rotor blade row. This eventually lowers the blade curvature and consequently also lowers the tendency for boundary layer growth and separation on the suction surface.

The flow features surrounding compressor blades are described in relatively greater detail in Test Case E/CO-1 by Serovy and Dring [114], Test Case E/CO-3 by Ginder and Harris [115] and Test Case E/CO-5 by Serovy and Dring [116] for the purpose of bench marking computational fluid dynamics codes. The blade camber angles used in the blade rows of the 3 relevant test cases are calculated across the span in the radial direction and shown in Table 5.1. The estimated blade angles from the stage un-stacking method are also well within this range.

Table 5.1. Span wise blade camber angles

Experiment	Blade row	Spanwise mean blade camber angle
Test Case E/CO-1	Rotor	51.81°
Test Case E/CO-3	Rotor	17.27°
	Stator	47.30°
Test Case E/CO-5	Rotor for stage 1 and 2	38.36°
	Stator for stage 1 and 2	43.78°

5.4 Acceptable range for stage degree of reaction

The analysis of the LM2500 gas turbine data in the present study shows stage degree of reaction is about 40% to 50%, with stage loading coefficient $\psi \approx 0.3$.

This may indicate that the initial LM2500 axial compressor design is guided by the RSRR approach (Mattingly [60]). Stage degree of reaction is a design choice as seen in axial compressor stage studies with high degree of reaction, such as Farmakalides et al. [117], and in studies with low degree of reaction, such as Qiang et al. [118]. In pursuing general guidelines for designing highly loaded axial compressor stages where $\psi \approx 0.65$, Dickens and Day [119] have concluded that increased stage reaction (>50%) is necessary to achieve maximum efficiency because the rotor blade losses are less severe than the stator blade losses. Noting the intricate interplay of stage loading, stage reaction and stage efficiency, should stage loading be the design objective, then stage reaction may be adjusted accordingly or vice versa.

5.5 Identifying the ignition temperature

The fuller ignition process occurs in stages. The simulation outcomes in Figure 4.20 show 3 distinct stages: a) no ignition, b) ignition only and c) ignition followed by a rapid temperature rise. As the foil temperature rises, more energy transfers to the reaction and progresses it to the next stage. Another 2 related stages are sustained combustion and extinction. However, the capability of the 2-step reaction to sustain combustion is not well demonstrated, as the available mesh is deemed unable to support the development of the vortices accompanying the rapid temperature rise (see Section 4.2.2).

According to the Van't Hoff ignition criterion, the "VIGR2" Arrhenius parameters narrow the ignition temperature to between 1300 K and 1310 K, which sits between 1252 K and 1367 K from Smyth and Bryner [1]. The "MILD2" Arrhenius

parameter set being much more reactive, indicates that the ignition temperature is likely far below 1300 K.

Since the “MILD2” Arrhenius parameters enable ignition at 1200 K, the ignition temperature obtained by this 2-step reaction mechanism may be tuned by using the “VIGR2” Arrhenius parameters with only small contributions from “MILD2” Arrhenius parameters in Equation (3.66).

However, the following implementation details have systematically placed the ignition temperature in a lower bracket. The 2-step reaction mechanism from Westbrook and Dryer [17] is a more reactive reaction mechanism compared to a detail reaction mechanism as no other intermediates and radicals form during the reaction. This implies that the identified ignition temperature bracket is likely lower than it should be. In addition, both radical quenching at the wall and heat loss to the wall are absent, making this a more reactive mechanism that identifies a lower ignition temperature. Again, this implies that the actual ignition temperature is higher. The adiabatic walls retain heat inside the domain, contributing to a more reactive reaction and underestimate the ignition temperature. Lastly the initial conditions used to test for the ignition temperature presents artificially higher initial concentrations of CH_4 and O_2 on the foil surface, since reaction are not enabled in the steady-state simulation used to prepare these initial values. These support the combustion reaction at a lower temperature, placing the ignition temperature in a lower bracket again.

Initially, it is intended to identify the ignition temperature to the nearest Kelvin. However, since the identified ignition temperatures are clearly above the maximum temperatures found in the last axial compressor stage of the LM2500, identifying the ignition temperature to the nearest 10 K is sufficient. This reaction mechanism is considered sufficient for use in future simulations to demonstrate that the conditions within the last compressor stage do not support hot surface ignition by the metallic surfaces.

5.6 Limitations due to the mesh

While keeping under the student node limit (512000), a number of problems occur. There are insufficient nodes to provide a fine grid in every part of the domain, the domain is shaped to focus only on the foil, locations away from the foil are filled with large cells and a 2D simulation domain is used to conserve nodes for the foil surface.

In this thin 2D simulation domain, the hot product gases from the reaction can only leave the foil surface by moving towards the domain edges. Since the expanding hot gases cannot move sideways (movement in the z direction), the gases also travel downwards within and outside the boundary layer to the beginning of the foil as seen in Figure 5.1. This strongly disrupts the incoming fresh methane-air mixture from reaching the foil and consequently the gas mixture temperature on the foil falls.

Figure 5.1. Expansion of hot product gases on the foil at 1400 K at time 0.004450 s

5.7 Implementing a detailed reaction mechanism

A clear shortcoming of the present implementation of 2-step reaction mechanism is the absent representation of radicals and intermediate species. A side effect of that is the temperature profile rises to its equilibrium flame temperature without slowing down as seen in the example in Figure 5.2. In comparison, the temperature profile obtained from CHEMKIN PREMIX rises rapidly then very gradually to the equilibrium temperature. These profiles are obtained from reactions under adiabatic conditions. The GRI-Mech 3.0 [83] reaction mechanism is used in CHEMKIN PREMIX.

Figure 5.2. Comparing Temperature vs time profiles between a 2-step and a detail reaction mechanism

The examples of more suitable temperatures vs. time profiles are shown in Figure 5.3, which are obtained from CHEMKIN PREMIX [120] using the GRI-Mech 3.0 [83] mechanism. Since equilibrium temperatures are not achieved immediately after the rapid temperature rise, such a reaction mechanism is not as reactive at the 2-step reaction mechanism.

Figure 5.3. Temperatures vs time profiles at equivalence ratio 0.7 obtained from CHEMKIN PREMIX [120] using the GRI-Mech 3.0 [83] mechanism.

The Computational Singular Perturbation (CSP) method summarises the essence of the detailed reaction mechanism into an equivalent reaction mechanism with a much smaller number of CSP-reactions [121]. The number of CSP-reactions is S . Suppose $S = 1$ is desired, this requires one $\vec{b}^s$ vector. The elements of the $\vec{b}^s$ vector could be viewed as a form of weightage used to select

the chemical species whose changes in mass fraction indicate the reaction progress. The lowercase “s” in the superscript refers to the slow reactions according to the CSP method.

A set of 1D freely propagating flame calculations is performed in J. Kok’s [120] version of PREMIX implemented at the University of Twente, for equivalence ratios 1.0 to as low as possible and initial temperatures from 273 K to 1800 K. The reaction mechanism is GRI-Mech 3.0 [83]. After applying the CSP process on these PREMIX outputs to obtain an equivalent 1 step CSP-reaction, a survey of the obtained $\vec{b}^s$ vectors shows this is the most common $\vec{b}^s$ vector (Equation (5.1) whose element values are recorded in Table 5.2), at all tested initial temperatures (273 K to 1800 K) and equivalence ratios 0.7 and greater.

$$\vec{b}^s = [b_{H_2} \quad b_H \quad b_O \quad \dots \quad b_{CH_2CHO} \quad b_{CH_3CHO} \quad b_{N_2}] \quad (5.1)$$

Subscripts indicate only the chemical species and the b values are shown in Table 5.2.

Table 5.2. A common CSP vector element values for initial temperatures 273 K to 1800K and equivalence ratios 0.7 and greater

Chemical species	Element value	Chemical species	Element value	Chemical species	Element value
H2	0.0	CH2OH	-1.5	NO2	0.5
H	0.5	CH3O	-1.5	N2O	1.0
O	1.0	CH3OH	-1.0	HNO	0.0
O2	1.0	C2H	-2.5	CN	-0.5
OH	0.5	C2H2	-3.0	HCN	-1.0
H2O	0.0	C2H3	-2.5	H2CN	-0.5
HO2	0.5	C2H4	-3.0	HCNN	-0.5
H2O2	0.0	C2H5	-2.5	HCNO	-1.0
C	0.0	C2H6	-3.0	HOCN	-1.0
CH	-0.5	HCCO	-0.5	HNCO	-1.0
CH2	-1.0	CH2CO	-3.0	NCO	-0.5
CH2(S)	-1.0	HCCOH	-3.0	AR	0.0
CH3	-1.5	N	0.5	C3H7	-4.5
CH4	-2.0	NH	0.0	C3H8	-4.0
CO	0.0	NH2	-0.5	CH2CHO	-2.5
CO2	0.0	NH3	-1.0	CH3CHO	-2.0
HCO	-0.5	NNH	0.5	N2	0.0
CH2O	-1.0	NO	0.5		

Generally, methane and oxygen are present in the summarised equivalent reaction mechanism. Water is not always present. Carbon dioxide, carbon monoxide, nitrogen and argon are absent.

The chemical species mass fraction vector $\vec{y}$, in the same order of species, is

$$\vec{y} = \begin{bmatrix} Y_{H_2} \\ \vdots \\ Y_{N_2} \end{bmatrix} \quad (5.2)$$

The CSP vector in this case has one only element η^s and

$$\eta^s = \vec{b}^s \vec{y} \quad (5.3)$$

The reaction progress variable c is

$$c = \frac{\eta^s - \eta^{s,UB}}{\eta^{s,EQM} - \eta^{s,UB}} \quad (5.4)$$

where $\eta^{s,UB} = \vec{b}^s \vec{y}^{UB}$ and $\eta^{s,EQM} = \vec{b}^s \vec{y}^{EQM}$. For superscripts, “UB” is for unburnt and “EQM” is for equilibrium. The source term for c is

$$S^c = \frac{1}{\eta^{s,EQM} - \eta^{s,UB}} \vec{b}^s \vec{y}^R \quad (5.5)$$

where $\vec{y}^R$ is the vector containing the net production of mass fraction for each species Y_i as the reaction progresses. The 1D transport equation for c is

$$\frac{dc}{dt} + u \frac{dc}{dx} = D \frac{d^2c}{dx^2} + S^c \quad (5.6)$$

In the present study, S^c is determined from $u(dc/dx)$ instead. The PREMIX outputs are in steady state so dc/dt is zero. The contribution of the diffusion term is tested to be negligible.

After determining the c and S^c at each time step, the raw S^c vs. c curve for combustion starting at 1400 K is shown in Figure 5.4A. To ensure smoothness,

3 functions are fitted resulting in the curve in Figure 5.4B. This S^c vs. c curve is not a continuous clean line due to accumulated slight discontinuities in the input values, which amplify when computing derivatives. The slight discontinuities arise, as precision in the PREMIX output text file is limited.

(A) S^c vs. c based on PREMIX output text file (B) S^c vs. c after decimating and curve fitting
Figure 5.4. Smoothing the reaction progress variable source term derived from PREMIX

For reactions to proceed, the initial S^c value must be positive and this value is heavily influenced by temperature in the Arrhenius rate equation. In a portion of the PREMIX outputs used, the reaction progress variable c is not always zero at the start of the 1D domain. An example of this is shown in Figure 5.5 where the PREMIX output obtained from an initial temperature 1400 K shows the fluctuating c values.

Figure 5.5. Fluctuating reaction progress variable values at the start of the 1D PREMIX domain

Within this set of PREMIX outputs, the initial c value is better behaved at lower initial temperatures and the distribution of initial c values, determined by fitting a hyperbolic tangent function, is applied to this set of premix outputs (Figure 5.6).

Figure 5.6. Adjusted reaction progress variable values at the start of the 1D PREMIX domain

The sensible enthalpy and c relationship when the combustion process starts at 1400 K is shown in Figure 5.7.

Figure 5.7. Sensible enthalpy vs. reaction progress variable

Each S^c vs. c and its corresponding h vs. c curve is for combustion starting at a specified initial temperature and only the reaction release more energy into the domain. In a hot surface ignition scenario, fresh pockets of methane-air mixture could meet other pockets of gas at various temperatures to gain energy and itself begin reacting to release more energy. This implies that a family of S^c vs. c

curves (Figure 5.8) and h vs. c curves (Figure 5.9) are required. Local enthalpy determines the curve to use.

Figure 5.8. A family of curves for source vs. reaction progress variable obtained from PREMIX and CSP

Since the maximum equivalence ratio is 0.7 and the pressure is 101325 Pa, S^c is function of only c and enthalpy in the present study.

Figure 5.9. A family of corresponding enthalpy vs. reaction progress variable

The relationship between a chemical species mass fraction and the c variable is shown in Figure 5.10 using the OH radical as an example. Similarly, the

required mass fraction curve is determined by the local specific static sensible enthalpy. The $S^c(c, h)$, and the 52 $Y_l(c, h)$ curves are communicated to the CFX software using the in-built 3D user functions.

Figure 5.10. A family of corresponding curves for OH radical mass fraction vs. reaction progress variable

For each species implemented in CFX, the NASA coefficients updated with data from the “thermo30.dat” file obtained from GRI-Mech 3.0 [83]. The molar masses are obtained from NIST websites [104], [105], [106], [107], [122], [123] and so on for all species in this reaction mechanism. Only 20% of the species are built from scratch and the other variables necessary for a complete specification of a material in CFX are gleaned from existing species in the CFX material library.

5.8 Applying the hot surface ignition results to the compressor

The stage un-stacking method is able to return a feasible axial temperature profile as seen in Figure 4.15. This profile shows that stages 15 and 16 attain a mean temperature of about 680 K and 723 K respectively. The hot surface

ignition temperature of methane-air mixtures flowing over small metallic surfaces, such as compressor blades in the last stages of the axial gas turbine and in the Smyth and Bryner [1] experiment, is 1300 K to 1310K. Noting that this bracket of ignition temperatures is underestimated, as explained in the previous section, the temperature buffer between the normally operating axial compressor and ignition temperature is at least 577 K (1300 K - 723 K) when speeds are at 0.16 m s^{-1} .

Of special note is that axial compressor operating at a maximum of about 723 K is well below 884 K, which is one of the lowest temperatures record to support ignition on a metal surface. This 884 K temperature comes from the experiment of Robinson and Smith [16], where their apparatus is a near spherical stainless steel container. Their experimental set up retains almost all the energy released by the methane reaction and ignitions take place only after 17-20 seconds. For an ignition scenario to take place within the studied axial compressor, the temperature must build up with almost no heat loss below while temperatures are below 884 K. These conditions will not be fulfilled as air is passing freely into and out of the axial compressor, transferring heat away. In addition, any heated expanding pocket of air is free to mix and disperse its heat.

In terms of temperature, this temperature buffer of at least 577 K and the lowest (no flow, near adiabatic) ignition temperature 884 K for methane over metal surfaces pose two great hurdles for an ignition scenario to develop in the axial compressor.

Under realistic LM2500 gas turbine wind down, the flow speeds are still high and far above 0.16 m s^{-1} . Due to forced convection, the metal surfaces will cool down rapidly and not maintain at 723 K. The high-speed air flowing past hot metal surfaces increases the ignition temperature and poses another hurdle for an ignition scenario to develop.

Therefore, the probability that an ignition scenario develops into a hot surface ignition within the axial compressor is considered very low. The follow on action of igniting a methane-air cloud within the last compressor stage and having this reaction burn through the methane-air cloud within the compressor until it reaches the rest of the methane-air cloud outside the gas turbine is considered unlikely.

5.9 A mechanism for probability of ignition

Babrauskas [124] ascribes a “probabilistic nature” to fire at the beginning of a very comprehensive ignition handbook. In the present study, the probability of ignition is considered by incorporating a probabilistic model into the combustion model only.

Several current combustion models are summarised by Versteeg and Malalasekera [125]. These approaches ensure combustion certainly takes place and the differences lie in the type of flow, degree of complexity and accuracy in representing combustion. However, these approaches prescribe ignition and are relevant to conditions conducive for combustion.

Within the resources of the present study, a 2-step reaction mechanism is implemented with a finite rate chemistry approach in the form of the Arrhenius rate equation. While the Arrhenius rate equation contains no probability aspects, this 2-step reaction mechanism supports a straightforward implementation of probability of ignition.

5.9.1 A subset of elementary reactions

Before determining probabilities, the 2-step reaction mechanism in the present study is shown to be at least possibly composed of one subset of elementary reactions from GRI-Mech 3.0 [83]. The overall reaction may be deliberately initiated by collisions of only O_2 and CH_4 molecules only and avoids radical chemical species acting on O_2 and CH_4 molecules. To improve clarity, bimolecular elementary reactions are selected as much as possible. When a termolecular elementary reaction is selected, the third body M (in Table 5.3) may be removed without affecting the reaction. This one possible subset of elementary reactions is summarised in Table 5.3. Other subsets are not explored. The elementary reactions are identified by their line number in the grimech30.dat file. Alternative elementary reactions are marked by “alt”.

Table 5.3. Selected GRI-Mech 3.0 [83] reactions that collapse into Westbrook and Dryer [17] 2-step reaction mechanism

Step	line number in <i>grimech30.dat</i> file	reaction	A [cm ³ mol ⁻¹ s ⁻¹ , cm ⁶ mol ⁻² s ⁻¹]	β []	E_a [cal mol ⁻¹]
A	196	$HO_2 + CH_3 \rightleftharpoons O_2 + CH_4$	1.00E+12	0.0000	0.0
B	62	$H + O_2 + N_2 \rightleftharpoons HO_2 + N_2$	2.60E+19	-1.2400	0.0
B-alt	63	$H + O_2 + Ar \rightleftharpoons HO_2 + Ar$	7.00E+17	-0.8000	0.0
C	243	$CH_3 + O_2 \rightleftharpoons OH + CH_2O$	2.31E+12	0.0000	20315.0
D	26	$O + H_2 \rightleftharpoons H + OH$	3.87E+04	2.7000	6260.0
E	40	$O + CH_2O \rightleftharpoons OH + HCO$	3.90E+13	0.0000	3540.0
F	176	$OH + HCO \rightleftharpoons H_2O + CO$	5.00E+13	0.0000	0.0
G	26	$O + H_2 \rightleftharpoons H + OH$	3.87E+04	2.7000	6260.0
H	64	$H + O_2 \rightleftharpoons O + OH$	2.65E+16	-0.6707	17041.0
I	156	$2OH \rightleftharpoons O + H_2O$	3.57E+04	2.4000	-2110.0
J	22	$2O + M \rightleftharpoons O_2 + M$	1.20E+17	-1.0000	0.0
K	56	$O_2 + CO \rightleftharpoons O + CO_2$	2.50E+12	0.0000	47800.0
K-alt	35	$O + CO(+M) \rightleftharpoons CO_2(+M)$	1.80E+10	0.0000	2385.0

The overall reaction starts with a collision of only O_2 and CH_4 molecules in step A. The HO_2 radical is used in both steps B and B-alt to give H radicals. The CH_3 radical from step A is used in step C to generate the OH radical. The resulting H and OH radicals are used in step D to produce H_2 . While step D has a lower A , the high β causes step D to proceed fast. The CH_2O radical is used in step E to generate HCO and OH radicals, which are quickly converted in step F to H_2O and CO .

The second water H_2O molecule may be obtained from the H_2 molecule through these reactions. The H_2 molecule is separated in step G to give a H radical. An additional O_2 molecule converts the H radical to a OH radical in step H. The 2 OH radicals produce H_2O in step I. The last 2 O radicals combine in step J to give O_2 , which is returned.

Collapsing elementary reactions from step A to J recovers step 1 of the 2-step reaction mechanism. Since some of the steps require using the elementary

reaction in reverse, the slow backward reaction rates support replacing the reversible reactions by an effectively irreversible reaction. Thus, step 1 of the 2-step reaction mechanism controls the reaction progress.

The $CO-CO_2$ equilibrium may be supported by steps K and K-alt. When the low probability collision with a third body M in step K-alt is removed, the pre-exponent increases. It helps to imagine that step K starts this equilibrium instead of K-alt. Step K-alt is step 2 of the 2-step reaction mechanism when the third body is removed.

5.9.2 Probability embedded in the reaction rate constant

The probability contribution embedded in the pre-exponent of step 1 is analysed according to the approach in Atkins and Paula [126]. A successful reaction depends on collision frequency of O_2 and CH_4 molecules in the correct orientation with sufficient energy. Comparing the empirical or experimental rate constant to the theoretical rate constant in Equation 22.13 of [126] gives

$$AT^{\beta} \exp\left(-\frac{E_a}{RT}\right) = \underbrace{P_{\text{STERIC}}}_{\text{steric factor}} \underbrace{\sigma_{CS} \left(\frac{8k_{\text{BM}}T}{\pi\mu_{\text{RM}}}\right)^{1/2}}_{\text{collision frequency}} \underbrace{N_{\text{AV}} \exp\left(-\frac{E_a}{RT}\right)}_{\text{sufficient energy}} \quad (5.7)$$

where σ_{CS} is the collision cross section and μ_{RM} is the reduced mass in atomic mass units. Applying Equation 22.3b of [126], the collision cross section for oxygen and methane is

$$\sigma_{CS} = \pi \left(\frac{d_{CH_4} + d_{O_2}}{2} \right)^2 \quad (5.8)$$

Applying Equation 22.3c of [126], the reduced mass for an oxygen and a methane in collision is

$$\mu_{RM} = \frac{M_{CH_4} M_{O_2}}{M_{CH_4} + M_{O_2}} \frac{1}{N_{AV}} \quad (5.9)$$

The probability of molecules colliding with the correct orientations is represented by P_{STERIC} and is a weak function of temperature.

Temperature dependence T^β is avoided by Westbrook and Dryer [17] when they determined the Arrhenius parameters of step 1 of their 2-step reaction mechanism. The rate constants marked as VIGR2 and MILD2 in Figure 5.11 come from rows 1 and 2 of Table IV in [17]. Temperature dependence is factored into the rate constants by adjusting the pre-exponent A so that the modified rate constant from the adjusted set of Arrhenius parameters matches closely the original rate constant as seen in Figure 5.11. The modified rate constants are marked VIGR2m and MILD2m respectively.

(A) Rate constant VIGR2 and VIGR2m

(B) Rate constant MILD2 and MILD2m

Figure 5.11. Factoring temperature dependence into the rate constants

While this choice of β is arbitrary, using $\beta=0.5$ completely removes the effect of temperature on P_{STERIC} . The 4 possible AT^β distributions obtained in Figure 5.11 are compared in Figure 5.12A to the collision frequency or theoretical pre-exponent for collisions of oxygen and methane and reveals that rate constants VIGR2 and VIGR2m imply more collisions than predicted. After removing the collision frequency in Equation (5.7), the 4 possible distributions of P_{STERIC} are shown in Figure 5.12B.

(A) AT^β as a function of temperature

(B) P_{STERIC} as a function of temperature

Figure 5.12. Removing collision frequency from pre-exponents

For the scenarios when $P_{STERIC} > 1$, the collision cross section is transformed into a larger effective collision cross section [126]. It is not that oxygen and methane molecules are not much more reactive or larger themselves but that the elementary reactions that make up this overall reaction involve radical species and are naturally fast reactions. This leads to a possibility that $P_{STERIC} = 1.0$ while σ_{CS} varies to model the highly reactive radicals.

However, in the present study, “VIGR2” Arrhenius parameters fit better the experimental data for ignition temperature. Since $P_{STERIC} > 1$, the VIGR2 and VIGR2m set may be used to build an ignition map. While the pre-exponents of the MILD2 or MILD2m set may support building an approximate ignition

probability map, the reactions are far too reactive and possibly removing the effects of reactions that momentarily do not proceed.

5.9.3 Effects of temperature and speed

The changes in the temperature field alter the frequency of molecules colliding. The transport of mass and momentum alter the flow field and mass fractions of reactants molecules. At the molecular level, the flow field consists of molecules in random motion. A successful reaction depends on molecules colliding and colliding with the correct orientation, leading to breaking their own bonds and reconstituting intermediates, radicals, main products or side products.

Reduced flow speed removes less heat and grants a larger proportion of the molecules sufficient energy to react. A larger surface area transfers more heat to more of the gas mixture. This leads to more pockets of gas undergoing their reactions and increases the chances of obtaining sufficient successful reactions that sustain stable heat release. The probability of ignition is repeatedly building upon (chain effect) the probability of successful reactions at the molecular level.

Chapter 6. CONCLUSIONS

At the time of the present study, a review of relevant existing standards, codes and rules, reveal that these do not address the possible scenario of flammable gas, such as methane, entering the gas turbine air intakes. There are also no membranes or filters that may perform rapid and efficient removal of methane from air. The gas turbine air intakes cannot shut out air from the external environment as the high-pressure spool is turning continually, drawing air in until the temperature becomes sufficiently low. The accepted engineering control is to prevent leaking flammable gas from coming into contact with gas turbine air intake. However, should flammable gas come into contact with hot surfaces inside the axial compressor, the extent of the temperature difference between the internal surfaces of a gas turbine compressor and the hot surface ignition temperatures indicates a measure of safety. Modelling this temperature difference requires the flow conditions within the axial compressor and a hot surface ignition chemistry model.

A stage un-stacking method is developed to realistically estimate stage temperature, stage pressure, stage axial velocities and flow angles within a multistage axial compressor operating at design point. The design options within this method are inferred from possible design guidelines that may be implemented in in-service gas turbines. The method implements iterative calculations to simultaneously fulfill thermodynamic requirements, velocity triangle requirements and user-selected design options at the mean line for the entire axial compressor.

The chemistry supporting hot surface ignition of methane-air mixtures at equivalence ratio 0.7 is successfully modelled by a finite rate implementation of a simple 2-step reaction mechanism by Westbrook and Dryer [17] for methane combustion. The Arrhenius rate equations set the reaction rates. Numerical implementation of this chemistry model in the Smyth and Bryner [1] experiment reveals that the ignition temperature, obtained only from gas phase chemistry, is between the 1300 K and 1310 K bracket. This range of ignition temperature is for flowing methane-air mixture at 0.16 m s^{-1} and lies within the 1252 K to 1367 K bracket in the experimental outcomes of Smyth and Bryner [1] at equivalence ratio 0.7 for stainless steel, titanium and nickel surfaces. The Van't Hoff ignition criterion indicates ignition on the heated surface when the temperature gradient moves from negative through zero to positive.

The highest temperature in the LM2500 compressor is 723.45 K. The minimum temperature difference between the normally operating axial compressor and ignition temperature is at least 577 K ($1300 \text{ K} - 723 \text{ K}$), assuming low speeds such as 0.16 m s^{-1} . Under actual wind down process, this temperature difference widens beyond 577 K as the surface temperatures fall with heat loss and the hot surface ignition temperature is much higher since flow speeds are far above the Smyth and Bryner [1] inlet speed 0.16 m s^{-1} . The reducing surface temperatures and much higher hot surface ignition temperatures indicate that hot surface ignition likelihood within the axial compressor is considered very low.

Chapter 7. FUTURE WORK

The Future work chapter identifies lacking aspects of the current set of simulation outcomes and more gas turbine specific information which the author considers helpful for building safety cases.

7.1 Building on the current set of simulation outcomes

The following aspects have yet to be explored in this set of simulations.

- A fuller 3D domain with boundaries located at far field – This avoids interrupting the proper formation of vortices near the heated foil.
- A refined mostly structured mesh throughout the domain – This supports the proper formation of vortices near the heated foil.
- Determining the ignition temperatures for gas mixtures at equivalence ratio 0.5 and below – This helps validate the use of a temperature only simulation approach for studying the combustion of lean pockets of methane-air mixture. Majority of the gas leaks are small gas leaks, which bring about only lean mixtures of methane in air.
- Exploring the effect of varying levels of turbulence intensity (1% to 20%) with the $k-\omega$ SST turbulence model – Increased turbulence at the foil surface is anticipated to dissipate more heat, requiring a higher surface temperature for ignition.
- Implementing other variations of $k-\omega$ SST turbulence model such as $k-\omega$ SST-sustain as mentioned by Rumsey [101] – This assesses the applicability of the combustion model for a wider range of common turbulent flow scenarios.

- Using a detailed mechanism – This results in a more accurate modelling of temperature during combustion and could indicate the extent of underestimation in the ignition temperature identified in the present study.
- Accounting for radical chemical activity on the wall - The modelling of surface reactions is required to determine a surface material's catalytic or quenching effect on ignition temperature.
- Improving the 1st SLC model to accept a local peak SLC at one of the front stages - The pressure ratios would peak in a similar manner shown in Figure 2.4 for the aero-derivative gas turbines, consistent with the next stage and clearly above 1. The axial velocity distribution is also expected to smoothen.

7.2 Pursuing gas turbine specific information

In the long run the following areas may be pursued so that supporting data at all phases of wind down and at all relevant parts of the gas turbine is available for more comprehensive simulations, which may be foundational in building safety cases. By developing as much of the gas turbine simulation independently, the platform operators are closer to proving to themselves that they increasingly fully understand their risks and are able to undertake greater independent decisions.

7.2.1 Transient gas turbine data

The potential of an ignition map may improve when both steady state and transient wind down of the compressor are analysed. This preliminary transient analysis uses only approximate data. The transient behaviours need to be

described by functions of time to specify the transient boundary conditions for simulations. The initial conditions are the steady state values before wind down.

Two sets of transient temperature data, which Pedersen [15] obtains within his research team, begin at the lower and upper temperatures found on the combustor casing. These are referred to as “TL” and “TU” in Figure 7.1A. The 3rd set of transient temperature data comes from Appendix D of [1] and is indicated by “TA” as it is only a temperature ratio applied on an arbitrary average temperature. After 30 minutes, the drop in temperature becomes gradual and tends to stabilize clearly above the ambient temperature. This is likely due to gas turbines being housed in enclosures, which restricts cooling air to only air drawn into the gas turbine by the turning of the high pressure spool. It is also possible for the high pressure spool to keep rotating slowly for a specified duration as part of the pre-defined wind down procedure, however this effect does not show up as a distinct phase in these temperature transients.

(A) Temperature transient (ss-steady state, amb-ambient)

(B) Rotating component wind down

Figure 7.1 Temperature and rotational speed transients in a LM2500 gas turbine during wind down

After some trial and error, the form of Equation (7.1) is found to fit the 3 available sets of transient temperature data for the time range 0 to 80 minutes (4800 seconds) in Figure 7.1A.

$$T = Ae^{-t^C/B} \quad (7.1)$$

The transient shaft rotational speed data indicated as “Compressor speed” in Figure 7.1B is from Wingerden [127] for a tripped gas turbine. The “Power turbine speed” and “Shaft power” data come from Appendix D of [1]. The power turbine winds down more quickly than the compressor as the power turbine is coupled to a load.

When wind down begins, the compressor has sufficient momentum to compress air for only a short duration. The resistance on the rotor is lower as the velocity

triangles are still maintained. As the wind down proceeds, the compressor eventually functions as a mixer. The flow becomes fully disrupted and the resistance on the rotor increases rapidly. Considering resistance at the bearings as negligible, the governing equation suggested for the shaft speed is

$$I_M \frac{d\omega}{dt} = -C_F \omega^n \quad (7.2)$$

where I_M is the moment of inertia and C_F is the coefficient of fluid resistance and the exponent n is a function of ω . This gives

$$\omega(t) = \begin{cases} [(C_F/I_M)(n-1)t + \omega_0^{1-n}]^{1/(1-n)} & , n \neq 1 \text{ and } n > 1 \\ \omega_0 \exp(t C_F/I_M) + \omega_{OFF} & , n = 1 \end{cases} \quad (7.3)$$

where $\omega_{OFF}=95.27 \text{ rad s}^{-1}$ when the “Compressor speed” data in Figure 7.1B begins at $912.67 \text{ rad s}^{-1}$. As compression gives way to mixing, each phase is described by Equation (7.3) with varying ω_0 , C_F/I_M ratio and n , found in Table 7.1.

Table 7.1. Shaft rotational speed coefficients for each phase of a compressor wind down for the LM2500

Phase of wind down	ω range	ω_0 [rad s ⁻¹]	C_F/I_M [kg m ² s ⁻²]/[s ⁻¹] ^b	n []	mass flow rate
Reducing compression	$\omega > 229.96$	912.67	4.827×10^{-3}	1.291	air is drawn in
Transition	NA	660.17	6.358×10^{-2}	1.000	flow stagnates
Mixing only	$\omega < 122.14$	198.43	1.084×10^{-1}	0.670	flow stagnates

This “Power turbine speed” data uses Equation (7.3) with $n > 1$. It must be noted that the transient mass flow rate is the last unavailable crucial information.

7.2.2 Flow conditions in a combustor

For the gas turbine in the present study, the steady state axial variation of combustor parameters may be found using the design approach of Mattingly et al. [9], but with a few small changes. In addition, 1D-isentropic relations are used to estimate the flow within the diffuser before the fuel atomizer and the

convergent transition duct after the dilution zone. The design approach in [9] is able to generate a sufficiently accurate approximate combustor geometry shown in Figure 7.2 that compares well with pictures of the LM2500 gas turbine combustor.

Figure 7.2 An approximate combustor geometry for the LM2500 gas turbine generated with the design approach of Mattingly et al. [9]

7.2.2.1 Dilution holes on the combustor liner and cooling air

A clear candidate for investigation are the flow structures formed by cooling air passing through the dilution and effusion holes on the combustor liner in the primary zone and secondary zone. These holes form a carpet of spots with slower flow and the temperature of air is above the accepted auto-ignition temperature of methane. Detailed geometry and flow field data is critical for determining the regions where slower flow may encourage unintended combustion and heat accumulation.

7.2.2.2 Flow conditions on the combustor liner

The design approach in [9] is applied as much as possible to the scant design information of the LM2500 gas turbine's combustor and results in the following initial estimates of temperature and axial flow speeds within the liner and outside (indicated by "Out") in Figure 7.3.

(A) Estimated temperature variations inside and outside the liner

(B) Estimated speed variations inside and outside the liner

Figure 7.3 Initial estimates of temperature and speed inside and outside the liner within an approximate combustor for the LM2500 gas turbine

7.2.3 Implementing probability for a reaction

The collision model for molecules is more appropriately applied to elementary reactions such as in Table 5.3, and P_{STERIC} is required for each elementary reaction. The interlinked nature of the elementary reactions, such as multiple pathway that may loop back, indicate no simple answer for the effective overall P_{STERIC} of the entire set of elementary reactions.

For each elementary reaction, the behaviour of colliding molecules is essentially isotropic. At each time step, in each control volume, the outcome of molecules colliding and thus, of the reaction could be obtained from picking a random number between [0,1] generated from a uniform distribution and compared to a criteria set up with P_{STERIC} .

7.2.4 An initial hot surface ignition map relevant to gas turbine conditions

To define an initial preliminary hot surface ignition map for the studied gas turbine, the 2 environments of the gas turbine to study are the last stages of the compressor and the combustor.

7.2.4.1 Simplifying the geometry

The primary flow path in a compressor may be predominantly approximated as flow through a rectangular duct. The flow paths within a combustor may be approximated as flow between parallel walls outside of the liner as seen in Figure 7.4 and flow through a circular duct within the liner. The common feature between these flow geometries is flow between parallel walls. A further simpler approximation of flow over a heated wall is not considered as this assumes a plane of symmetry between the parallel walls.

Figure 7.4. Approximation of the LM2500 combustor liner into duct flow

7.2.4.2 Worst case flow conditions

For ingesting flammable gas during normal operation, an analysis of the ignition process needs to be carried out at high pressure and at high speed, in addition to other conditions listed in Table 7.2. For the last stages of the compressor, Klapproth et al. [11] reports the mean axial speed and Pedersen [15] reports the wall temperature. The combustor design approach by Mattingly et al. [9] is used

to estimate the axial variations of pressure, mean speed and wall temperature for the primary and secondary zones inside the combustor.

Table 7.2. Approximate conditions during normal operation of a LM2500 gas turbine

Normal operation	Overall pressure	Mean speed	Wall temperature
Last stages of compressor	19 atm	114 m s ⁻¹ [11]	800 K [15]
Combustor primary and secondary zones	19 atm [9]	40 m s ⁻¹ [9]	1172 K [9]

For ingesting flammable gas during wind down, an analysis of the combustion process is done from high to atmospheric pressure and from high to low speed, in addition to other changes in conditions listed in Table 7.3. Once the gas turbine has almost wound down, the mass flow rate of air drifting through due to convection is low. If the mass flow rate is 3 kg s⁻¹, the mean speed is 44 m s⁻¹ in the last stages of the compressor and 10 m s⁻¹ in the combustor primary and secondary zone. The compressor is assumed to wind down to standard reference conditions, as stated in BS ISO 3977-2:1997 [88].

Table 7.3. Approximate change in conditions within the last stages of the compressor and combustor as a LM2500 gas turbine shuts down

Shut down process	Overall pressure	Mean speed	Wall temperature
Last stages of compressor (descriptive rate of change)	19 to 1 atm (very rapid)	114 to 44 m s ⁻¹ (rapid)	800 to 278.15 K (slow)
Combustor primary and secondary zones (descriptive rate of change)	19 to 1 atm (very rapid)	40 to 10 m s ⁻¹ (rapid)	1172 to 278.15 K (slow)

7.2.5 A high pressure flow hot surface ignition experiment

Ignition temperatures obtained in high pressure, flowing, hot surface ignition experiments are lacking as such experiments are highly resource intensive. With valuable inputs from Dr. Jim B. W. Kok (University of Twente), a suggested test section for such experiments is shown in Figure 7.5. The test section has a heated metallic inner surface over which a mixture of air and methane flows. The reaction may be observed through a side quartz glass optical access.

Figure 7.5. A possible high pressure flow test section for hot surface ignition

7.2.6 Secondary flow system of a gas turbine

The secondary flow system of a gas turbine extracts high pressure air from the compressor at a middle stage or at the outlet to support internal cooling of turbine blades. The path way taken by the extracted air is unlike that in the primary flow and instead has many corners and turns within the blade and inside the hub. Such corners and turns are necessary for enhanced heat transfer from the hot turbine blades into the cooler extracted air, however, they are also possible locations to accumulate heat leading to ignition should the extracted air be contaminated with methane.

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