Department of Precision and Microsystems Engineering

Evaporative Two-Phase Micro-Flow Modelling

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Evaporative Two-Phase Micro-Flow Modelling

A study of Vaporizing Liquid Microthrusters

by

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As smaller satellites hold many advantages over their larger counterparts, such as reduced production, testing and launch costs, the cubesat standard of very small satellites has become increasingly popular over the last decade.

For these cubesats (1 to 3 kg) the race for an adequate yet simple propulsion system is on, as traditional exothermic rocket engines cannot be easily scaled down to appropriate sizes.

Vaporizing liquid micro-thrusters (VLM) are a promising solution to provide reliable thrusters, as the principle combines the tried and proven inert-gas thruster systems with the dense and compact storage of liquids. The liquids are evaporated using an external heating source, and the consequently created vapour is accelerated through a nozzle structure to provide thrust. However, in the design of VLM systems little two-phase fluid-flow modelling has been performed so far.

Multi-phase fluid flow is a challenging area in the field of fluid dynamics. The analytic evaporation models published so far focus on high mass-flux (> 100[kg m\(^{-2}\) s\(^{-1}\)]) cooling of integrated circuits, and are restricted to low vapour fraction (< 0.2) operation to maximise the silicon-cooling potential of the fluid flow.

By contrast, VLM systems require all of the fluid to be evaporated for optimal performance, resulting in unity vapour mass fractions. To ensure full evaporation, low mass-flux (< 30[kg m\(^{-2}\) s\(^{-1}\)]) systems are generally used. This mismatch ensures that evaporation models cannot be freely exchanged.

It is the goal of this thesis to further the knowledge in modelling of evaporative two-phase flows in microstructures, to be able to improve the design methods of VLM’s.

This thesis therefore presents two methods of investigating two-phase fluid flow behaviour, novel to VLM design-studies. They will be implemented on the current state of art VLM design by the TU Delft, both as a test case for the methods, and to investigate possible design improvements.

Firstly an analytical modelling approach is presented, correlated using visual data available in published literature. Secondly a first-principle modelling approach is presented, using a newly-developed adaptation of the Reynolds equation, with a reintroduction of both inertia terms and viscous friction terms of in-plane fluid motion.

The analytical approach is shown to provide insight in design improvement options, and is expected to be a valuable tool in the future design methodology of VLMs, allowing for the identification of minimal wall temperatures, efficiency values and performance values of VLM designs. The first-principle approach, solved using numerical means, shows promise, as it reduces the computation time of two-phase fluid flow systems drastically compared to the reference of the phase-field method. Future work on the stabilisation of the numerical algorithms is still required.

This thesis will conclude with a set of recommendations based on the performed simulations, enabling designers to improve current VLM design strategies.
Getting here, to the point where I can present my Master of Science Thesis, I have walked a winding path. In 2006, at the University of Utrecht, I started my first Bachelor program in Medicine. Fast forward to 2010, and upon graduating with my BSc. in Medicine, I was duly fed up with my studies.

At that point, I choose to follow my dream and restart my scientific education with a Bachelor's degree in Mechanical Engineering. Just over five and a half years later, I present this thesis as the capstone to my MSc. of Mechanical Engineering.

After completing my work as an intern at Volvo Cars in Sweden, in the final study year of my MSc, Urs Staufer guided me to find Barry Zandbergen and his wish to create reliable, cheap and efficient propulsion systems for very small satellites.

Taken under the wings of both Barry Zandbergen and Ron van Ostayen, I was able to dive into the inner workings of two-phase evaporative micro-fluid systems, and see what was already there, what was needed, and what could be done.

This work before you has seen numerous counts of frustration, balanced by counts of sudden successes. Even though not all of the goals we set out to complete were successfully attained, I am proud of what we have accomplished.

We set out to both create analytical models to test current propulsion designs, and numerically-solved first-principle based models, to investigate the possibilities of numerical optimisation in evaporative two-phase flow systems. In my naive understanding of the latter method, I assumed that most of my time would be spent on assessing the underlying optimisation procedures. I was proven wrong.

Instead this work presents the intended analytical models, correlated to published data, as well as a new approach and set of equations to describe thin-film-like evaporative flows.

I hope that this new method can give rise to future developments and, perhaps, numerical optimisation of said two-phase flow phenomena, so that the design methods on numerical optimisation that are being pioneered in the department of Precision and Micro-system Engineering can be extended to this domain as well.

I am very grateful for the guidance I received from my professors, and similarly grateful for the many critical discussions I’ve had the pleasure of conducting with my fellow students!

I would be remiss not to thank my parents, for allowing me to make such a drastic restart-decision, and to support me while I extended my study period to nine and half years.

I’m happy to find my girlfriend still by my side, who started out dating a would-be-doctor, and ended up putting up with a near-indefinite student!

Many others have helped me during my efforts, with words of advice, an interested question, or specified criticism. You are too many to mention, but each and every contribution is appreciated.

So without further ado, please enjoy my thesis!

Caspar Antonius Jacobus Hanselaar
Delft, March 2016
The object of study requires a wide array of models, and similarly a wide array of variables. All symbols used in this thesis are listed below. First Latin and Greek variables are shown in tables 1 and 2. Next constants are shown in table 3. Mathematical constructs are summarised in table 4, and indices used in table 5.

<table>
<thead>
<tr>
<th>symbol</th>
<th>Unit</th>
<th>Physical quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>a</td>
<td>[m s(^{-1})]</td>
<td>speed of sound</td>
</tr>
<tr>
<td>(A_{x_1})</td>
<td>[m(^2)]</td>
<td>Cross-sectional area perpendicular to direction (x_1)</td>
</tr>
<tr>
<td>Bo</td>
<td>[1]</td>
<td>Bond number</td>
</tr>
<tr>
<td>C</td>
<td>[m s(^{-1})]</td>
<td>Evaporation mass flux speed tuning parameter COMSOL</td>
</tr>
<tr>
<td>(C_{rd})</td>
<td>[1]</td>
<td>Discharge ratio for a real vs. ideal nozzle</td>
</tr>
<tr>
<td>Co</td>
<td>[1]</td>
<td>Confinement number</td>
</tr>
<tr>
<td>(e_p)</td>
<td>[J kg(^{-1}) K(^{-1})]</td>
<td>Specific isobaric heat</td>
</tr>
<tr>
<td>(C_{tp})</td>
<td>[1]</td>
<td>Two-phase region heat transfer coefficient</td>
</tr>
<tr>
<td>(e_v)</td>
<td>[J kg(^{-1}) K(^{-1})]</td>
<td>Specific volumetric heat</td>
</tr>
<tr>
<td>(D_h)</td>
<td>[m]</td>
<td>Hydraulic diameter</td>
</tr>
<tr>
<td>(D_p)</td>
<td>[m]</td>
<td>Hydraulic diameter of pillars</td>
</tr>
<tr>
<td>(e)</td>
<td>[J kg(^{-1}) K(^{-1})]</td>
<td>Specific enthalpy</td>
</tr>
<tr>
<td>(e_{LIH})</td>
<td>[J/kg]</td>
<td>Specific latent heat</td>
</tr>
<tr>
<td>F</td>
<td>[N]</td>
<td>Force (or thrust-force)</td>
</tr>
<tr>
<td>G</td>
<td>[kg m(^{-2}) s(^{-1})]</td>
<td>Mass flux</td>
</tr>
<tr>
<td>(g)</td>
<td>[N kg(^{-1})]</td>
<td>Body force per unit of mass</td>
</tr>
<tr>
<td>h</td>
<td>[W m(^{-2}) K(^{-1})]</td>
<td>Heat flux coefficient</td>
</tr>
<tr>
<td>(I_{sp})</td>
<td>[1]</td>
<td>Specific impulse</td>
</tr>
<tr>
<td>(I_x)</td>
<td>[m(^4)]</td>
<td>Second moment of inertia</td>
</tr>
<tr>
<td>Kn</td>
<td>[1]</td>
<td>Knudsen number</td>
</tr>
<tr>
<td>(\Delta H)</td>
<td>[1]</td>
<td>Mach number</td>
</tr>
<tr>
<td>m</td>
<td>[kg]</td>
<td>Mass</td>
</tr>
<tr>
<td>(\dot{m})</td>
<td>[kg s(^{-1})]</td>
<td>Mass flow</td>
</tr>
<tr>
<td>Nu</td>
<td>[1]</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>(\mathcal{P})</td>
<td>[m]</td>
<td>Perimeter</td>
</tr>
<tr>
<td>P</td>
<td>[W]</td>
<td>Power</td>
</tr>
<tr>
<td>p</td>
<td>[Pa]</td>
<td>Pressure</td>
</tr>
<tr>
<td>Q</td>
<td>[W]</td>
<td>Heat flow rate</td>
</tr>
<tr>
<td>(Q_{gen})</td>
<td>[W m(^{-3})]</td>
<td>Heat generation per unit of volume</td>
</tr>
<tr>
<td>(q')</td>
<td>[W m(^{-2})]</td>
<td>Heat flux</td>
</tr>
<tr>
<td>R</td>
<td>[m]</td>
<td>Local radius of curvature</td>
</tr>
<tr>
<td>Re</td>
<td>[1]</td>
<td>Reynolds number</td>
</tr>
<tr>
<td>(S)</td>
<td>[1]</td>
<td>Slip ratio of vapour vs. liquid speed</td>
</tr>
<tr>
<td>T</td>
<td>[K]</td>
<td>Temperature</td>
</tr>
<tr>
<td>t</td>
<td>[s]</td>
<td>Time</td>
</tr>
<tr>
<td>(\mathbf{u}_3)</td>
<td>[m s(^{-1})]</td>
<td>Velocity vector (3D) of fluid</td>
</tr>
<tr>
<td>(\mathbf{u}_{2})</td>
<td>[m s(^{-1})]</td>
<td>Height-averaged velocity (2D) of fluid</td>
</tr>
<tr>
<td>(\mathbf{u})</td>
<td>[m s(^{-1})]</td>
<td>Longitudinal (duct) velocity (1D) of fluid</td>
</tr>
<tr>
<td>(\mathbf{u}_d)</td>
<td>[m s(^{-1})]</td>
<td>Superficial (duct) velocity (1D) of fluid</td>
</tr>
<tr>
<td>V</td>
<td>[m(^3)]</td>
<td>Volume</td>
</tr>
<tr>
<td>(\nu_{vf})</td>
<td>[1]</td>
<td>Volume fraction of vapour</td>
</tr>
<tr>
<td>(x_{vf})</td>
<td>[1]</td>
<td>Mass fraction of vapour</td>
</tr>
</tbody>
</table>

Table 1: Latin symbols used in this thesis
<table>
<thead>
<tr>
<th>symbol</th>
<th>Unit</th>
<th>Physical quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>α</td>
<td>[1]</td>
<td>Phase indicator</td>
</tr>
<tr>
<td>γ</td>
<td>[1]</td>
<td>Specific heat ratio</td>
</tr>
<tr>
<td>ΔV</td>
<td>[m s$^{-1}$]</td>
<td>Delta-V budget</td>
</tr>
<tr>
<td>ε</td>
<td>[1]</td>
<td>Fraction of space not occupied by pillars in heater</td>
</tr>
<tr>
<td>η</td>
<td>[1]</td>
<td>Emittance</td>
</tr>
<tr>
<td>η$u$</td>
<td>[1]</td>
<td>Efficiency</td>
</tr>
<tr>
<td>θ</td>
<td>[s]</td>
<td>Residence time</td>
</tr>
<tr>
<td>κ</td>
<td>[W m$^{-1}$ K$^{-1}$]</td>
<td>Conductivity</td>
</tr>
<tr>
<td>λ</td>
<td>[m]</td>
<td>Free path length of gas molecules</td>
</tr>
<tr>
<td>μ</td>
<td>[Pa s]</td>
<td>Viscosity</td>
</tr>
<tr>
<td>ρ</td>
<td>[kg m$^{-3}$]</td>
<td>Density</td>
</tr>
<tr>
<td>σ</td>
<td>[N m$^{-1}$]</td>
<td>Surface tension</td>
</tr>
<tr>
<td>ε</td>
<td>[m]</td>
<td>Interface thickness</td>
</tr>
<tr>
<td>ϑ</td>
<td>[s]</td>
<td>Residence time</td>
</tr>
<tr>
<td>κ</td>
<td>[W m$^{-1}$ K$^{-1}$]</td>
<td>Conductivity</td>
</tr>
<tr>
<td>λ</td>
<td>[m]</td>
<td>Free path length of gas molecules</td>
</tr>
<tr>
<td>μ</td>
<td>[Pa s]</td>
<td>Viscosity</td>
</tr>
<tr>
<td>ρ</td>
<td>[kg m$^{-3}$]</td>
<td>Density</td>
</tr>
<tr>
<td>σ</td>
<td>[N m$^{-1}$]</td>
<td>Surface tension</td>
</tr>
<tr>
<td>ε</td>
<td>[m]</td>
<td>Interface thickness</td>
</tr>
<tr>
<td>ϑ</td>
<td>[s]</td>
<td>Residence time</td>
</tr>
<tr>
<td>κ</td>
<td>[W m$^{-1}$ K$^{-1}$]</td>
<td>Conductivity</td>
</tr>
<tr>
<td>λ</td>
<td>[m]</td>
<td>Free path length of gas molecules</td>
</tr>
<tr>
<td>μ</td>
<td>[Pa s]</td>
<td>Viscosity</td>
</tr>
<tr>
<td>ρ</td>
<td>[kg m$^{-3}$]</td>
<td>Density</td>
</tr>
<tr>
<td>σ</td>
<td>[N m$^{-1}$]</td>
<td>Surface tension</td>
</tr>
<tr>
<td>ε</td>
<td>[m]</td>
<td>Interface thickness</td>
</tr>
</tbody>
</table>

Table 2: Greek symbols used in this thesis

<table>
<thead>
<tr>
<th>symbol</th>
<th>Unit</th>
<th>Physical quantity</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Rs</td>
<td>[J kg$^{-1}$ K$^{-1}$]</td>
<td>Specific gas constant for water</td>
<td>461.9</td>
</tr>
<tr>
<td>$k_{sb}$</td>
<td>[W m$^{-2}$ K$^{-1}$]</td>
<td>Stefan-Bolzmann constant</td>
<td>5.67 · 10$^8$</td>
</tr>
<tr>
<td>F</td>
<td>[1]</td>
<td>Vandenkerckhove function</td>
<td>0.67, unless otherwise specified</td>
</tr>
<tr>
<td>$g_0$</td>
<td>[m s$^{-2}$]</td>
<td>Gravitational acceleration at sea level</td>
<td>9.81</td>
</tr>
<tr>
<td>$N_A$</td>
<td>[mol$^{-1}$]</td>
<td>Avogrado number</td>
<td>6.022 14 · 10$^{23}$</td>
</tr>
<tr>
<td>$M$</td>
<td>[kg kmol$^{-1}$]</td>
<td>Molar mass water</td>
<td>18</td>
</tr>
</tbody>
</table>

Table 3: Constants used in this thesis

<table>
<thead>
<tr>
<th>Operator</th>
<th>Action</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\nabla_n$</td>
<td>($\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_2} + ... + \frac{\partial}{\partial x_n}$), or the spatial derivate to $n$ spatial dimensions</td>
</tr>
<tr>
<td>⊗</td>
<td>Dyadic, using the Cartesian coordinate system synonymous with the outer product of two vectors</td>
</tr>
<tr>
<td>$I$</td>
<td>Identity tensor</td>
</tr>
<tr>
<td>$x,y,z$</td>
<td>Coordinate system directions</td>
</tr>
<tr>
<td>$n$</td>
<td>Normal vector to indicated surface area</td>
</tr>
</tbody>
</table>

Table 4: Math operators observed that might be unclear to the reader
<table>
<thead>
<tr>
<th>Index</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>V</td>
<td>Indicating quantity refers to a vapour</td>
</tr>
<tr>
<td>L</td>
<td>Indicating quantity refers to a liquid</td>
</tr>
<tr>
<td>t</td>
<td>Indicating quantity refers to the nozzle throat plane</td>
</tr>
<tr>
<td>e</td>
<td>Indicating quantity refers to the nozzle exit plane</td>
</tr>
<tr>
<td>c</td>
<td>Indicating quantity refers to the final heater-chamber values</td>
</tr>
<tr>
<td>w</td>
<td>Indicating quantity refers to a wall</td>
</tr>
<tr>
<td>u</td>
<td>Indicating quantity refers to the velocity</td>
</tr>
<tr>
<td>fb</td>
<td>Indicating quantity refers flow-boiling</td>
</tr>
<tr>
<td>cfb</td>
<td>Indicating quantity refers convective flow-boiling</td>
</tr>
<tr>
<td>nfb</td>
<td>Indicating quantity refers nucleate flow-boiling</td>
</tr>
<tr>
<td>IRT</td>
<td>Indicating quantity refers to convective Ideal Rocket Theory</td>
</tr>
<tr>
<td>real</td>
<td>Indicating quantity refers to realistic measurements</td>
</tr>
<tr>
<td>evap</td>
<td>Indicating quantity refers to evaporation</td>
</tr>
<tr>
<td>Si</td>
<td>Indicating quantity refers to Silicon</td>
</tr>
<tr>
<td>SiC</td>
<td>Indicating quantity refers to Silicon Carbide</td>
</tr>
<tr>
<td>ext</td>
<td>Indicating quantity refers to exterior of system</td>
</tr>
</tbody>
</table>

Table 5: Table detailing indices used in this thesis

On index numbering referring to spatial systems: in this thesis the convention is maintained that the first spatial index (1) refers to the longitudinal direction. The second index (2) indicates a direction perpendicular to the first direction, but still horizontal, positive using the right hand rule. The final index (3) indicates the height-dimension, perpendicular to the first to indices.
# Contents

1 Introduction .......................... 1
   1.1 Thruster design .......................... 2
      1.1.1 Thruster concepts .......................... 2
      1.1.2 Current design and modelling .................... 3
      1.1.3 Modelling methods available .......................... 3
   1.2 Goal of Thesis .......................... 3
      1.2.1 Opportunities for design .................. 3
      1.2.2 Modelling methods assessed .......................... 4
   1.3 Thesis structure .......................... 4

2 Fundamentals .......................... 5
   2.1 Single phase flow .......................... 6
      2.1.1 Navier-Stokes equations .......................... 6
      2.1.2 Thin film flows .......................... 8
      2.1.3 Duct flows .......................... 8
      2.1.4 Heated flow .......................... 9
   2.2 Nozzle flows and thruster performance .......................... 10
      2.2.1 Specific Impulse and delta-V budget .......................... 10
      2.2.2 Ideal Rocket Theory .......................... 10
   2.3 Macroscopic two-phase evaporation .......................... 13
      2.3.1 Pool boiling .......................... 13
      2.3.2 Flow boiling .......................... 14
      2.3.3 Macro flow-boiling models .......................... 15
      2.3.4 Discerning macro-scale boiling from micro-scale boiling .......................... 16
   2.4 Microscopic two-phase evaporative flow .......................... 17
      2.4.1 Micro-flow-boiling behaviour .......................... 17
      2.4.2 Behaviour specific to VLM’s .................... 20
      2.4.3 Current micro-flow-boiling models .......................... 20
   2.5 VLM designs and modelling .......................... 21
      2.5.1 Current designs .......................... 21
      2.5.2 Current modelling employed .......................... 21
   2.6 Chapter summary .......................... 22

3 Analytical models .......................... 23
   3.1 Methods of heat transfer .......................... 23
      3.1.1 Direct wire to fluid heating .......................... 24
      3.1.2 Wire through silicon to fluid heating .......................... 24
   3.2 Fragility of heating wires .......................... 25
   3.3 Reverse-flow restrictions .......................... 26
   3.4 Energy-balance model .......................... 27
      3.4.1 Mass flow rate calculation .......................... 27
      3.4.2 Fluid power requirements .......................... 28
      3.4.3 Propellant efficiencies .......................... 32
      3.4.4 Energy-balance model in review .......................... 33
   3.5 Steady-state 1D flow model .......................... 33
      3.5.1 Approach .......................... 34
      3.5.2 1D time-averaged algorithm .......................... 34
      3.5.3 Preliminary results .......................... 35
      3.5.4 Correlations with experimental data .......................... 37
      3.5.5 Results of correlated time-averaged 1D model .......................... 39
3.5.6 Silicon temperature gradient ............................................................. 41
3.5.7 Effects of rhombi on fluid flow .......................................................... 42
3.5.8 Simulation results of rhombi-model ...................................................... 44
3.5.9 Silicon temperature gradient (rhombi case) .......................................... 46
3.5.10 Review of time-averaged 1D model .................................................... 47
3.6 Transient 1D flow model ........................................................................... 48
3.6.1 Transient 1D model algorithm ............................................................... 48
3.6.2 Results of transient 1D model ............................................................... 51
3.6.3 Review of transient 1D model ............................................................... 51
3.7 Conclusions on analytical modelling ......................................................... 52

4 First-principle based model studies ............................................................ 55
4.1 First-principle model scenario’s ................................................................. 55
4.2 COMSOL phase-field approach ............................................................... 57
4.2.1 Conservation of momentum and mass ................................................. 57
4.2.2 Finding the interface ............................................................................. 58
4.2.3 Interface equations ............................................................................... 58
4.3 Phase-field results .................................................................................... 60
4.3.1 Abstract model simulations ................................................................. 60
4.3.2 Real system simulations ....................................................................... 60
4.3.3 Computation time ............................................................................... 62
4.3.4 Review of the phase-field method ....................................................... 62
4.4 Simplications of physics .......................................................................... 63
4.4.1 Surface tension simplification ............................................................... 63
4.4.2 Evaporation region simplification ....................................................... 63
4.5 Initial Reynolds-model results ................................................................. 65
4.6 Analysis of model instabilities .................................................................. 66
4.6.1 Physics of the difficulties ..................................................................... 66
4.6.2 Temperature and pressure field oscillations ......................................... 67
4.6.3 Applied stabilisation methods .............................................................. 68
4.7 Adjusted physics results .......................................................................... 69
4.7.1 Navier-Stokes results ......................................................................... 69
4.7.2 Real system simulations ...................................................................... 70
4.8 Conclusions on first-principle modelling ............................................... 71

5 Conclusions and Recommendations ........................................................ 73
5.1 Conclusions ............................................................................................. 73
5.1.1 Modelling ........................................................................................... 73
5.1.2 Design ................................................................................................. 74
5.2 Recommendations ................................................................................... 74
5.2.1 Modelling ........................................................................................... 74
5.2.2 Design ................................................................................................. 74

Bibliography ....................................................................................................... 77

A Poyck VLM design ....................................................................................... 81
A.1 VLM: Operation ....................................................................................... 81
A.2 VLM: design. ........................................................................................... 82
A.3 Other designs ........................................................................................... 84
A.4 VLM Dimensions .................................................................................... 84
A.5 VLM Material .......................................................................................... 85
A.6 VLM: Performance figures ...................................................................... 86
A.7 Continuum theory .................................................................................. 86
A.8 VLM mounting and operation. ................................................................. 87

B Creating phase-transfer models ................................................................. 89
B.1 Correlation-based modelling .................................................................... 89
B.2 First-principle modelling .......................................................................... 91
B.3 Appendix summary ................................................................................. 96
C Analytical model results .................................................. 97
  C.1 Reynolds numbers ..................................................... 97
  C.2 Flow Velocities ...................................................... 97
D Water Properties ............................................................. 103
  D.1 Balance model ......................................................... 103
  D.2 1D steady state model ............................................... 103
  D.3 1D transient model .................................................. 104
  D.4 First-principle models .............................................. 104
E Reducing the 3D Navier-Stokes equation ................................. 105
  E.1 Limitations to the 2D reduction ..................................... 106
  E.2 Qualitative and Quantitative comparison .......................... 107
  E.3 Conclusions .......................................................... 110
F Predictive Analytical model (paper contribution Space Propulsion 2016) .................................................. 111
  F.1 Abstract (relevant addition) ......................................... 111
  F.2 Method ........................................................................ 111
  F.3 Results ....................................................................... 112
  F.4 Conclusion of contribution ............................................. 113
  F.5 Discussion of contribution ............................................. 113
  F.6 Glossary ..................................................................... 114
H Analytical models ............................................................... 117
  H.1 Balance model ............................................................ 117
  H.2 Steady-State model ...................................................... 120
  H.3 Transient 1D model .................................................... 126
Currently cubesats are en vogue: a wide variety of academic institutes and commercial parties have expressed the intention to launch, or have already launched their cubesat projects [1]. The term cubesat refers to a very small subset of satellites, built to a fixed set of design criteria concerning outside dimensions and mass, and restrictions concerning the use of various potentially harmful materials such as pyrotechnics or pressurised systems.

Cubesats have several advantages: due to their limited size very large conventional satellite testing facilities are no longer necessary, launch payloads are greatly reduced allowing for smaller launch vehicles to be used, or even allowing for a piggy-back-ride with another launch. Companies like NanoRacks have set up delivery systems for a large number of cubesats simultaneously, as shown by their launch of cubesats from the ISS.

![Figure 1.1: Artist impression of the DelFFi mission in progress, a tandem flight of two cube-sat type satellites. Each satellite has a mass of $\approx 3$[kg] and a volume of $\approx 3$[dm$^3$]. Image adapted from [2].](image)

New difficulties arise in miniaturising satellites to cubesats: all satellite subsystems and scientific equipment must be miniaturised as well. The cubesat standard prescribes dimensions of 1.33 kg per 1U (cubesat standardised unit, in effect a cube of exactly one cubic decimetre) [3]. This entails a high level of integration
between subsystems [4], posing its very own design challenges next to the already tough challenges of designing spacecraft.

### 1.1. Thruster Design

Satellite capabilities such as velocity control are often left out of cubesat designs due to relatively large size and mass requirements of thruster systems. Such penalties are very hard to bear in a 1 to 3 U cubesat, as it limits the space left for other mission critical systems. However the importance of the inclusion of such thruster systems is illustrated by the fact that nearly all large-scale satellites incorporate thruster systems [5].

The TU Delft plans to launch a cubesat mission, in coordination with the global QB50 mission (in 2016). This mission specifies research of low earth orbit (LEO) and subsequent slowed re-entry over a prolonged period of time [6]. As such, a propulsion system is essential to be able to complete the mission goals. Despite the long list of cubesat launches, the number of cubesats that have successfully operated a propulsion system in space is very limited. So far, in order of date of operation that list includes CanX-2, Delfi-n3Xt, POPSAT-HIP 1, CanX-4/5 and BRICsat-P [1, 7].

#### 1.1.1. Thruster Concepts

To provide an efficient thruster system, the following relevant performance criteria are to be met [8].

<table>
<thead>
<tr>
<th>Requirement</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thrust</td>
<td>0.5 - 9.5 [mN]</td>
</tr>
<tr>
<td>Velocity change ($\Delta V$)</td>
<td>$&gt;15$ [m/s]</td>
</tr>
<tr>
<td>Operational life</td>
<td>1 [year]</td>
</tr>
<tr>
<td>On-off cycle count</td>
<td>$&gt;5000$</td>
</tr>
<tr>
<td>System mass</td>
<td>$&lt;0.459$ [kg]</td>
</tr>
<tr>
<td>Heating power</td>
<td>$&lt;10$ [W]</td>
</tr>
<tr>
<td>Maximum internal pressure</td>
<td>$&lt;10$ [bar]</td>
</tr>
</tbody>
</table>

Table 1.1: Requirements for the propulsion system

Of the requirements, the required velocity change, or $\Delta V$ budget begs some explaining. Given the thrust levels attained per unit of propellant, and a total system mass (expected to be $\approx 3$ [kg]), the possible acceleration is calculated, using Newton’s second law. Given the total available propellant, the propulsion system is only able to fire for a finite amount of time. Therefore, the acceleration attained with the thruster, integrated over the time that it is able to fire due to propellant availability, provides the total possible velocity change, or the $\Delta V$ budget of the mission.

As it is infeasible to scale down conventional thruster systems, the in-house development of a micro-sized propulsion system commenced at the TU Delft with the work of Tittu Matthews in cooperation with Marco Mihailovic, and their heated ‘cold’-gas thruster built with MEMS technology [4, 9]. The term ‘cold’-gas refers to an inert gas being used as propellant, in contrast to exothermic reactions in propellants used in large-scale thrusters. [9] found a 30% reduction in propellant usage due to the heating of the gas was possible, whilst attaining the same thrust levels.

Based on the ‘technology-readiness-level’ of ‘commercial of the shelf’ (COTS) alternatives investigated by [5, 8, 10], the development of a resistojet project has continued [10].

As storing sufficient propellant in gaseous form to attain the $\Delta V$ budget is difficult given the 10 [bar] pressure constraint (see table 1.1), using a liquid propellant and subsequently evaporating it utilises the relatively low-pressure and high mass density storage of a liquid, while still having enough propellant available to attain the $\Delta V$ budget. Consequently to maximise efficiency of propellant use, it is important to ensure full evaporation in the VLM. More details on the importance of this will be presented in chapter 2. This type of evaporating-liquid thruster is often referred to as a vaporizing liquid micro-thruster (VLM).
1.1.2. CURRENT DESIGN AND MODELLING

So far the designing efforts in the TU Delft have produced several thruster concepts [4, 11], making the TU Delft a forerunner in VLM development. However, limited modelling effort is currently spent in designing these systems, comprised mainly of the heat required to evaporate the envisioned mass flow, and mass flow calculations for the nozzle, based on the ideal rocket theory [10, 11] and CFD analysis [10].

The most recent design iteration is calculated to have a thrust range of 0.8 to 1.4 [mN], a mission-specific ∆V of 21.01 [m/s] whilst using an expected power of less than 6.8 [W], with a mass flow rate of approximately 1 [mg/s] [8].

Pressure drop calculations for the heater-system are performed using a packed-bed based calculation, using the adjusted Ergun-equation [12]. The concluded expected pressure drop in the heater section of the VLM thruster of \(1.28 \times 10^5\) [Pa] [8] begs critical note, as based on a re-iterated calculation using the same values, a pressure drop of 201 [Pa] is predicted. (This equation will be detailed in chapter 3.)

These doubts concerning pressure drops, as well as the limited modelling performed on other aspects, leaves an assessment of the distribution of the heating power in the system uncompleted, nor does it compute expected power efficiencies. Modelling could furthermore be used to shed light on the two-phase flow, and any possibility of incomplete evaporation and subsequent reduction in propellant use efficiency.

1.1.3. MODELLING METHODS AVAILABLE

Several authors have published their work concerning the development of VLM’s. However modelling efforts reported in these publications are limited. Of those who published their modelling efforts [13] show a quick analytical model able to produce required heating power and expected steady-state thrust levels, while [14] reports a dry-heated (heat analysis without propellant present) analytical model to estimate pre-heat time required. Furthermore [15] and [16] used CFD computations of single phase flow through the nozzle like the research performed at the TU Delft by [10], while most other authors use the ideal rocket equations for thrust estimations.

None of the VLM-related publications known to the author of this thesis investigated two-phase flow behaviour or modelling, nor have they attempted simulations of these flows.

1.2. GOAL OF THESIS

It is apparent that current designs have not been modelled sufficiently to assess expected performance, nor is it possible to perform design improving studies with the current models, nor have others published relevant results detailing such modelling efforts with respect to VLM’s.

The goal of this project is therefore two-fold: firstly to efficiently model two-phase evaporative flows in micro-structures, taking into account not just the flow and evaporation effects, but also the surrounding structure, and secondly to use these models to improve the current design and future design strategies for VLM’s.

1.2.1. OPPORTUNITIES FOR DESIGN

Being able to model two-phase evaporative flows will allow the engineer to check for design flaws and the possibility for undesired flow patterns to arise in the VLM. Next, the ability to model such flows allows for the possibility of numerical optimisation techniques to be applied to two-phase flows and the heater structure.

The questions that are to be answered with these models are:

1. What is the expected power efficiency of the system?
2. What is the expected propellant efficiency of the system?
3. What is the expected power distribution in the heater based on a uniform wall temperature?
4. Given a heater dimension and pressure, what is the required wall temperature to ensure evaporation?
5. What dynamic two-phase flow effects specific to VLM’s can be identified?
Using the answers to these questions, desired design changes can be identified suggesting the final question of this thesis:

6. What design improvements can be proposed based on the model results?

1.2.2. Modelling methods assessed

To model two-phase flows, two main modelling approaches are evaluated:

- Analytical modelling of two-phase flows
- First-principle numerically solved modelling of two-phase flows

Of the stated modelling approaches, the analytical approach yields considerable insight into the basics of the evaporation process, yet is very hard to extend beyond a 1D approach. Despite this drawback, questions 1, 2 and 3 are expected to be sufficiently answered using analytical models. Questions 4 and 5 are expected to be partially assessed.

First-principle modelling allows for extra insight into the systems behaviour, as less assumptions and simplifications are required, when compared to analytical models. It is unfortunately more difficult to implement. COMSOL Multi-physics is applied for this approach.

It is expected that the numerical approach can provide much more detail on question 5, and might allow for the most versatile design improvements. To that end the option to use the numerical models for a topology optimisation study is investigated.

1.3. Thesis structure

In chapter 2 the fundamental equations concerning fluid flow and heat transfer will be discussed, as well as the effects of boiling, both in macroscopic as in microscopic systems. Next, in chapter 3 a discussion of used modelling techniques in current VLM design, and opportunities for better modelling are discussed.

Chapter 3 will use this knowledge to provide analytical models capable of answering questions 1 through 3 posed in section 1.2.1, while they will also provide an initial assessment of questions 4 and 5, for VLM designs similar to the current design by [11], whilst concluding with the identifiable design improvements.

Chapter 4 will provide an investigation of numerical methods able to model two-phase flows in micro-structures similar to the current VLM design, to assess if further insight and design improvements are identifiable.

Finally chapter 5 will provide concluding remarks, and assess the matter of completion of the thesis goals.
The subject of Vaporizing Liquid Micro-thrusters, despite the riveting sound of that name, begs some extra introduction. In figure 2.1, the two main subjects of this thesis are shown (albeit abstractly). In figure 2.1a, silicon base structure is seen, that forms the backbone of the VLM. At 1, you see the inlet channel, 2 indicates the heater chamber and 3 indicates the integrated convergent-divergent nozzle structure.

General operation using figure 2.1a is as follows: liquid enters the system at index 1, is heated at in the chamber (2.) until evaporation, and then some more (ideally), and exits through the nozzle (3) to space, where the nozzle causes the vapour flowing through to gain some extra speed.

That operation-diagram indicates that in order to say anything meaningful on the subject of modelling the internals, we need to identify 4 regions shown in figure 2.1b:

1. Single phase, heated flow. Entering the chamber (in liquid form), this is the process that needs to be initially understood.

2. Two-phase, heated and evaporating flow. Here a careful study of two-phase theory and micro-system fluid behaviour is required to be able to model it correctly.

3. Single phase, heated flow (this time vapour instead of liquid).

4. Nozzle flow calculations, comprised of acceleration of the fluid up to the local velocity of sound, and subsequent continued acceleration.

Note that section 1 and 3 are very much alike, save for a marked shift in properties. The borders where each of the described regions end, and new ones begin, is mostly blurry and ill-defined. Due to the soon-to-be-described unpredictable flow patterns in micro-flow systems, interface locations cannot be pre-assigned, but
must be computed by models.

In contrast to the open-chamber configuration shown in figure 2.1a, the preferred design by \[11\] uses small silicon pillars with a diamond-shaped cross-section, as seen in figure 2.2. These pillars support silicon-carbide resistance heater wires, spanning the width of the chamber. These wires are hypothesised by \[8\] to increase the efficiency of the system by reducing heat-losses through the silicon base structure to the satellite frame, and increase heat transfer to the liquid efficiency.

According to \[8\], the expected thrust range is 0.8 to 1.4 [mN], whilst using less than 6.8 [W], with a mass flow rate of approximately 1 [mg/s] or less, or a mass flux of 2.22[kg/m²·s] in the main heater section, for a design where the heater-chamber is approximately 9 [mm] in length, the width is approximately 3 [mm], and the height is 0.15 [mm]. Pressures in the storage tank are expected to vary between 0.5 and 5.5 [bar] (absolute pressure), and consequently the feed-pressures into the heater will vary accordingly, as the system operates in blow-down mode (fluid flow is generated using a pressurised tank, and due to the flow of fluid out of the tank, this pressure is gradually reduced during mission life). The liquid propellant is designed to be pressurised using a flexible bladder within a rigid tank. Please see appendix A for further details, such as initial Reynolds numbers estimates, showing a laminar flow structure based on average flow speeds throughout the system, and Knudsen numbers, showing that even in the lower pressure case, the system up to the nozzle's throat can still very much be considered a continuum system, as opposed to a discontinuous gaseous system.

In this chapter, first the principles governing liquid single-phase flow will be covered (section 2.1). Next, a brief summary of the principles used for the nozzle-flow calculations, as well as terms needed to judge thruster performance, will be provided (section 2.2), before finally introducing the background necessary to create two-phase evaporative flow models for macroscopic systems (section 2.3), and finally microscopic models (section 2.4).

2.1. SINGLE PHASE FLOW

This section will first introduce a general description for fluid flow and heating, the Navier-Stokes equation. Subsequently, a simplification usable for thin-film flows is introduced in section 2.1.2. Next, heat-transfer simplifications that are simultaneously employed are introduced.

2.1.1. NAVIER-STOKES EQUATIONS

Derived by Stokes and Navier independently, the so-called Navier-Stokes equations have been used to describe fluid flow since the early 1800’s. These equations must be valid for a sufficiently small volume of fluid, but one sufficiently large such that individual atoms don’t disrupt the continuous behaviour of the fluid. The equations are based on three main principles:

1. No mass may appear or disappear spontaneously
2. Momentum must be conserved, ergo a change of speed is due to a non-zero net force
3. No energy may spontaneously appear or disappear
This is expressed in compact form in equations 2.1 to 2.3:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}_3) = 0 \tag{2.1}
\]
\[
\frac{\partial (\rho \mathbf{u}_3)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_3 \otimes \mathbf{u}_3 + p \mathbf{I}) = \nabla \cdot \mathbf{F} + \rho \mathbf{g} \tag{2.2}
\]
\[
\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot \left( (\rho c_p T) \mathbf{u}_3 \right) - \nabla \cdot (\kappa \nabla T) = Q_{\text{gen}} + \mathbf{F} \cdot \nabla \mathbf{u}_3 \tag{2.3}
\]

In these equations, several new symbols are introduced: density \(\rho\) [kg m\(^{-3}\)], time \(t\) [s], 3D velocity \(\mathbf{u}_3\) [m s\(^{-1}\)], pressure \(p\) [Pa], shear stress \(\mathbf{F}\) [Pa], body force per mass (for instance gravitational acceleration) \(\mathbf{g}\) [N kg\(^{-1}\)], isobaric heat capacity \(c_p\) [J kg\(^{-1}\) K\(^{-1}\)], temperature \(T\) [K], the conductivity \(\kappa\) [W m\(^{-1}\) K\(^{-1}\)] and generated heat \(Q_{\text{gen}}\) [W m\(^{-3}\)].

Furthermore, several new short-form notation methods are introduced: \(\nabla_3\), indicating the spatial derivative in three dimensions, \(\mathbf{I}\), the identity matrix.

As this thesis deals with relatively slow moving fluids in the VLM heater (the nozzle is excluded here), the heating of the fluid due to viscous friction is neglected. Furthermore this viscous friction term is simplified using the notion that we are investigating a Newtonian fluid, meaning that the viscous stresses arising from heating of the fluid due to viscous friction is neglected. Furthermore this viscous friction term is simplified using the notion that we are investigating a Newtonian fluid, meaning that the viscous stresses arising from heating of the fluid due to viscous friction is neglected.

Equation 2.4 and the notion of dealing with slow-moving fluids simplifies equations 2.2 to 2.5 and equation 2.3 to 2.6, respectively:

\[
\frac{\partial (\rho \mathbf{u}_3)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_3 \otimes \mathbf{u}_3 + p \mathbf{I}) = \rho \nabla^2 \mathbf{u}_3 \tag{2.5}
\]
\[
\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot \left( (\rho c_p T) \mathbf{u}_3 \right) - \nabla \cdot (\kappa \nabla T) = Q_{\text{gen}} \tag{2.6}
\]

Though these equations should be able to describe any fluid motion, they are best applied to laminar flows. These flows are described as non-mixing flows, with Reynolds numbers of approximately 1000 or less [17, 18]. Reynolds numbers are calculated using equation 2.7:

\[
\text{Re}_D = \frac{\rho u D_h}{\mu} = \frac{\dot{m} D_h}{A_{cs} \mu} \tag{2.7}
\]

Note that here \(u\) represents the average local velocity magnitude: a 1D value. The term \(\dot{m}\) is the mass flow rate [kg s\(^{-1}\)], while \(D_h\) represents the hydraulic diameter, or the equivalent diameter if the system were circular. It is calculated using equation 2.8, where \(\mathcal{P}\) represents the wetted perimeter (in this case \(\mathcal{P} = 2W + 2H\)):

\[
D_h = \frac{A_{cs}}{\mathcal{P}} \tag{2.8}
\]

Given initial estimates of a mass flow rate of \(\dot{m} = 1\) [kg s\(^{-1}\)], hydraulic diameter of \(D_h = 2.9 \times 10^{-4}\) [m] and cross-sectional area of \(A_{cs} = 4.5 \times 10^{-7}\) [m\(^2\)], for liquids using a viscosity of \(\mu = 1 \times 10^{-3}\) [Pa s] the estimated Reynolds number is \(=0.63\), while for gases using a viscosity of \(\mu = 1.6 \times 10^{-5}\) [Pa s] the estimated Reynolds number is \(=32\), both clearly laminar. It is therefore safe to assume that the entire studied process is a laminar flow process.
2.1.2. THIN FILM FLOWS

The current design investigation deals with a thin VLM design: the height dimension is about a factor 20 smaller than the width dimension, and a factor 67 smaller than the length dimension. For the sake of convention in this thesis, please see figures 2.1a and 2.2 for the application of the coordinate system: $x_1$ is the direction pointing along the length of the heater, $x_2$ points in the horizontal plane to the width of the heater, while $x_3$ represents the height-dimension (see appendix A for further details).

Any vertical fluid motion will therefore be much smaller than any horizontal movement. In 1886 an approach exploiting this very small dimension was suggested by Osborne Reynolds [19], while [20] extended the usage of this Reynolds Equation to a more general description.

In this Reynolds equation, some simplifications are included:

1. The fluid is a Newtonian fluid, indicating that viscous forces are linear to the strain rate.
2. Inertia and body force terms are negligible compared to pressure forces and viscous forces, meaning velocity changes are instantaneous. This is reminiscent of Stokes flow, where viscous forces dominate and inertia forces are negligible [17].
3. Due to the small height compared to the other dimensions, derivations with respect to the height of the fluid film are considered much greater.
4. There is no slippage between fluid and wall at a boundary

The following assumptions are also included specific to this thesis:

5. For any horizontal position (ergo, on the length-width plane), the fluid properties throughout the local height are uniform
6. Both top and bottom fluid boundary (the heated walls) are at stand-still: they are defined to have no horizontal and no vertical movement

These assumptions will allow us to pose equation 2.9 as a measure of the pressure distribution, with $H$ the height in the system.

$$\nabla^2 \left[ \frac{\rho H^3}{\mu} \nabla^2 p \right] = H \frac{\partial \rho}{\partial t} \quad (2.9)$$

Equation 2.9 reduces the number of variables that define the flow field, as instead of a decoupled velocity and pressure distribution, now only a pressure distribution is to be calculated, and the velocity distribution is a direct result of the pressure distribution.

As suggested, the fluid is only allowed to move in the horizontal plane according to this formulation. This reduces the dimensions for computation form 3D to 2D: the function term $\nabla^3$ is reduced from $\nabla^3$ to $\nabla^2$. Furthermore, equation 2.9 can be used to determine the height-averaged horizontal speeds ($u_2$, in 2D) as a function of the local pressure gradient, as seen in equation 2.10:

$$u_2 = -\nabla^2 p \frac{H^2}{12\mu} \quad (2.10)$$

Equation 2.9 can effectively replace equations 2.1 and 2.5, reducing the quadratic function implied in the inertia forces to a linear second order differential function.

2.1.3. DUCT FLOWS

When systems can be further reduced to single-dimension systems, computation time is further reduced. However, this comes at the cost of information. For instance for the current VLM design, the relatively large width is ignored in a 1D approximation, and any important flows in that direction will not be accounted for.

To allow this kind of computation, material properties will have to be averaged over both the height (as in section 2.1.2), as well as the width of the flow. Furthermore, assuming steady-state behaviour of the system, the pressure drop over a section can be calculating by rewriting equation 2.10 for a single dimension, as seen in equation 2.11:
\[ \frac{\partial p}{\partial x} = -u \frac{12\mu}{H^2} \quad (2.11) \]

Using a known or specified mass flow rate, the velocity can be computed using equation (2.12):

\[ u = \frac{\dot{m}}{\rho A_{cs}} \quad (2.12) \]

### 2.1.4. Heated Flow

Instead of solving the full third Navier-Stokes equation (2.6), in analytical approaches often a reduced method is applied: Newton’s law of cooling. This method uses a local heat transfer coefficient \( h \) [W m\(^{-2}\) K\(^{-1}\)], a surface temperature \( T_w \) [K], and the local mean fluid temperature \( T \) [K], to calculate the heat flux into the fluid \( q''_w \) [W m\(^{-2}\)] (2.13).

\[ q''_s = h(T_w - T) \quad (2.13) \]

As we are discussing a mean temperature, this implies that we compressed the information on certain dimensions. For a duct (1D), the mean temperature implies averaged over the cross-section \( A_{cs} \), while for a thin film flow (2D) it implies averaged over the height of the flow \( H \). To investigate the total heat influx into the fluid, equation (2.13) will have to be multiplied with the conducting area in question.

Meanwhile the local convective heat transfer coefficient has been found to depend on several parameters [18]:

- Flow cross-section shape
- Reynolds number of the flow
- Hydraulic diameter of the flow

Equation (2.14) is used to calculate the local heat transfer coefficient [18]:

\[ h_{\text{conv}} = Nu \frac{\kappa}{D_h} \quad (2.14) \]

Nusselt numbers (\( Nu \)) are a function of Reynolds numbers, Prandtl, and possibly viscosity and the friction coefficient [18]. However, for laminar flows, the Nusselt number primarily depends on the shape of the duct cross-section, with tabulated values for each cross-section available in [18]. When ignoring the heat-flux enhancing pillars, and studying the VLM as depicted in figure 2.1a, Nusselt numbers in the order of 6.0 are appropriate according to [18].

The reduced energy equation is a simplified from of equation (2.6), where at least one in-plane dimension is prescribed by the existing part of the equation, and the out-of-plane dimensions are represented by the addition of the equation (2.13), where \( T \) is understood to be the mean fluid temperature. For a 2D flow study, this results in equation (2.15), while for a 1D study it results in equation (2.16), where \( \partial \) is the change of the perimeter of the section of the duct.

\[ \frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot ((\rho c_p T)u) - \nabla \cdot (\kappa \nabla T) = Q_{\text{gen}} + h(T_s - T) \quad (2.15) \]

\[ \frac{\partial (\rho c_p T)}{\partial t} + \frac{\partial}{\partial x} ((\rho c_p T)u) - \frac{\partial}{\partial x} \left( \kappa \frac{\partial T}{\partial x} \right) = Q_{\text{gen}} + h(T_s - T) \partial \quad (2.16) \]

Equation (2.15) generally lends itself to finite element or finite volume calculations, though it might also be solvable using analytical means for a limited (non-phase-change) subset of problems, while equation (2.16) is solvable using analytical means.
2.2. NOZZLE FLOWS AND THRUSTER PERFORMANCE

The VLM under investigation is intended to operate on a cube-sat in lower-earth-orbit (LEO) [6]. As such, some performance figures need to be calculated, such as the previously introduced $\Delta V$ budget. As such, this section will introduce another performance metric (specific impulse and $\Delta V$ budget), and calculations referring to section 4 of figure 2.1b: the ideal rocket theory (IRT).

2.2.1. SPECIFIC IMPULSE AND DELTA-V BUDGET

The specific impulse is a measure of the propellant efficiency. This provides the ratio of force delivered over mass flow of propellant and the standard gravitational acceleration at sea level:

$$I_{sp} = \frac{F}{mg_0}$$  \hspace{1cm} (2.17)

Consequently, the units of the specific impulse are s, and it is not a dimensionless property. Nonetheless it is often used to judge the thruster performance. Values of approximately 270[s] are typical for conventional rocket engines, according to [21], while [15] suggest specific impulse values for the current state-of-art of VLM design to vary between 50 and 105[s].

Higher $I_{sp}$ values indicate more efficient use of propellant mass: using a smaller amount of propellant, the same force can be exerted. Given a finite amount of propellant available in the spacecraft, this boils down to a certain time (based on the available propellant) that the thruster can provide a force on the spacecraft.

This finally results in a key measure introduced first in chapter 1, the $\Delta V$ budget. To ascertain the manoeuvrability of spacecraft, it will need to be able to change its velocity. For instance the goals of the QB50 mission state a controlled re-entry from LEO into the atmosphere. This indicates that due to the increasing friction of the atmosphere that will be encountered, numerous velocity changes will have to be executed.

It can be readily understood that the thrust available, divided by the mass of the vehicle, results in the acceleration. Multiplying this factor over the time that the thruster is able to work due to the available propellant, results in a crude measure for the $\Delta V$ budget, as seen in equation 2.18:

$$\Delta V = \frac{Ft}{m_{vehicle}}$$  \hspace{1cm} (2.18)

As propellant mass is often a significant portion of the vehicle in spacecraft, and thruster force may vary during operating life, a better measure is to include those effects, as seen in equation 2.19:

$$\Delta V = \int_0^t \left( \frac{F(t)}{m_{vehicle}(t)} \right) dt$$  \hspace{1cm} (2.19)

2.2.2. IDEAL ROCKET THEORY

The ideal rocket theory, or IRT, is a 1D model approximation to judge mass flow through a choked de Laval nozzle, a firstly converging and, after a minimal cross-section point, diverging duct [21]. Note that for this derivation it is assumed that the fluid flowing through the nozzle is fully evaporated, and can be described using the ideal gas law (IGL):

$$p = m \frac{R_s T}{V} = R_s \rho T$$  \hspace{1cm} (2.20)

Here $V$ represents the local volume of the fluid, $m$ the mass in question, and $R_s$ the fluid-specific gas constant, calculated as the universal gas constant divided by the molar mass of the gas, amounting to $\approx 461.9[J kg^{-1} K^{-1}]$. In keeping with the ideal gas assumptions, the specific heats are held constant, and as such the ratio $\gamma = \frac{c_p}{c_v}$ is similarly constant. To accommodate calculations, a value of 1.3 is used for $\gamma$, as suggested by [17] for the temperature and pressure range in question for water vapour. The specific isobaric heat is assumed to be $2100[J kg^{-1} K^{-1}]$, unless otherwise specified. See appendix D for more details on fluid properties used, as well as a short description of assumptions relating to the ideal gas law.
Assuming an isentropic process, the energy balance for a fluid can be set up as in equation 2.21, with \( e [\text{Jkg}^{-1} \text{K}^{-1}] \) the specific enthalpy in the fluid, and indices indicating two different locations (x and y), instead of dimensions as previously used.

\[
e_1 - e_2 = \frac{1}{2} (u^2_2 - u^2_1) = c_p (T_1 - T_2)
\]  

(2.21)

When we assume that the velocity of the fluid is negligible in the heating chamber of the VLM (section 2 in figure 2.1a), an expression relating the local velocity in the nozzle to the local temperature and chamber (starting) temperature can be set up, as seen in equation 2.22:

\[
T_c = T + \frac{u^2}{2c_p}
\]  

(2.22)

Here the subscript \( c \) represents the final chamber value, in this case the final chamber temperature \( T_c \).

The ideal gas law and subsequent thermodynamic relations are used to rewrite temperature in terms of pressure or volume via equation 2.23:

\[
\frac{T_1}{T_2} = \left( \frac{p_1}{p_2} \right)^{\gamma - 1} = \left( \frac{V_1}{V_2} \right)^{\gamma - 1}
\]  

(2.23)

The relation between stagnation pressure and local pressure can be extrapolated, using equations 2.21 and equation 2.23:

\[
p_c = p \left( 1 + \frac{u^2}{2c_p T} \right)^{\gamma - 1}
\]  

(2.24)

It is assumed that the velocity in the throat of the nozzle lies at the local speed of sound, referred to as a chocked flow. The local speed of sound is determined in equation 2.25:

\[
M = \frac{u}{a} = \frac{u}{\sqrt{\gamma R_s T}}
\]  

(2.25)

The ‘Mach’ is subsequently defined as the ratio of the local velocity to the speed of sound. As we are considering chocked flows, the relation between stagnation temperature, local temperature and Mach number can be assessed as [21]:

\[
T_c = T \left( 1 + \frac{\gamma - 1}{2} M_e^2 \right)
\]  

(2.26)

Consequently, using a similar method to equation 2.26, the local pressure can be correlated to the Mach number:

\[
p_c = p \left( 1 + \frac{\gamma - 1}{2} M^2 \right)^{\gamma}
\]  

(2.27)

As the area ratio between two points can be expressed as the ratio between the Mach numbers, for any arbitrary position, these can be chosen as the throat area (with known Mach number of 1) and the exit plane:

\[
\frac{A_e}{A_t} = \frac{1}{M_e^\gamma} \left( \frac{1 + [\gamma - 1] M_e^2}{1 + [\gamma - 1]} \right)^{\gamma/2}
\]  

(2.28)

Rewriting equation 2.28 allows the determination of the expected Mach speed at the exit plane. Knowing the Mach number, and computing the local temperature using equation 2.26, the local exit velocity is computed using the inverted equation 2.25:
Similarly, a relationship for the exhaust velocity as a function of chamber pressure to outside (nozzle exit, denoted by subscript $e$) pressure can be set up [22]:

$$u_e = M_e \sqrt{R_s T_c}$$  \hspace{1cm} (2.29)

Using similar principles, an expression for mass flow through the nozzle can be created:

$$\dot{m} = \frac{p_c A_t \Gamma}{\sqrt{R_s T_c}}$$  \hspace{1cm} (2.31)

Here in equation 2.31 $A_t$ represents the cross-sectional area of the smallest area of the nozzle, while the Vandenkerckhove function ($\Gamma$) represents a function dependent on the specific heat ratio ($c_p/c_v$):

$$\Gamma = \sqrt{T_c} \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma - 1}{2(\gamma - 1)}}$$  \hspace{1cm} (2.32)

The IRT model is based on an axisymmetric 1D nozzle, so the planar nozzle implemented in the current-design VLM will have lower mass throughput due to the boundary layer obstructing a larger portion of the cross section, as the perimeter to cross-sectional area ratio increases for planar nozzles [22]. This effect is described using the discharge fraction $C_d$, calculated in equation 2.33:

$$C_d = \frac{\dot{m}_{\text{IRT}}}{\dot{m}_{\text{real}}}$$  \hspace{1cm} (2.33)

Consequently, a more realistic mass flow is calculated as:

$$\dot{m} = C_d \frac{p_c A_t \Gamma}{\sqrt{R_s T_c}}$$  \hspace{1cm} (2.34)

As measurements of the VLM design are as of yet unavailable, the mass flux is estimated using a computational fluid dynamics (CFD) study, performed by [10]. His study showed that the mass flow was an average of 20% lower in the CFD study compared to the IRT-calculated values. Furthermore, he noted that surface roughness can induce another loss up to about 20%. As such, the ejection values are estimated to be 0.7 for the purpose of this study, which is in line with experimentally determined discharge values for nozzle flows with Reynolds numbers less than 500, according to [4].

Using the data generated by the IRT model, a thrust estimate can be calculated. The intended working condition of the VLM is the vacuum of space, therefore the thrust generated by the nozzle is calculated by equation 2.35, where $A_e$ represents the nozzle cross-sectional area at the exit to space. Note that to calculate a measure for $u_e$ and $p_e$, the Mach number $M_e$ is required. This value is determined by numerically solving equation 2.28, where the Mach number is the area ratio's are known. This value for $M_e$ can subsequently be used to calculate $u_e$ and $p_e$ using equations 2.29 and equation 2.27.

$$F_{\text{IRT}} = \dot{m} u_e + A_e p_e$$  \hspace{1cm} (2.35)

However, next to the reduced mass flow rate due to the boundary layer in the throat of the nozzle, the velocity of the fluid at the exit plane is similarly non-uniform, due to the boundary layers in the rest of the divergent part of the nozzle. As such, a CFD study performed by [15] is studied, who showed that the fluid is able to attain the calculated exit velocity only in approximately approximately 55% of the cross-sectional area of the exit plane of the nozzle (see figure 2.3). Extrapolating to a quadratic decreasing function in the boundary layer, which yields an average flow velocity of 2/3 of the free-stream velocity in the boundary layer, the following expression for the average exhaust velocity is generated:
\[ \eta_u = \left( 0.55 + 0.45 \cdot \frac{2}{3} \right) = 0.85 \] (2.36)

This velocity efficiency \( \eta_u \) amounts to 85% of the original exhaust speed. These findings are in agreement with the conclusions by [23]. Recomputing the expected force generated results in equation (2.37).

\[ F_{\text{RT}} = \eta_u (\dot{m}u_e) + A_e p_e \] (2.37)

2.3. **MACROSCOPIC TWO-PHASE EVAPORATION**

This section refers to fluid section 2. indicated in figure 2.1b. Even though the small dimensions of the VLM under investigation hint at a microscopic-sized boiling process, this section will first expand on the knowledge needed to understand the general principle of boiling and evaporation, by investigating macroscopic boiling processes. Initially in section 2.3.1 the general evaporation case of ‘saturated pool boiling’ is used to explain the basic boiling and evaporation behaviour, while section 2.3.2 will detail what the introduction of a forced flow changes to the process of boiling, while section 2.3.3 will introduce a commonly used model, which exemplifies the structure of most macroscopic flow boiling models. Next, section 2.3.4 will indicate when the limits of macroscopic models are reached, and when the need arises to switch to microscopic boiling models, which will be detailed in the next main section 2.4.

2.3.1. **POOL BOILING**

As summarised by [18], saturated pool boiling (meaning: the bulk of the fluid is at or slightly above saturation (boiling) temperature) consists of four phases (see figure 2.4): first the natural convection phase, where no vapour bubbles detach from the surface, which can be maintained up to about \( \approx 5\,[\text{K}] \) of superheat at atmospheric pressures [18]. Due to slight density changes of the liquid, the (lighter) heated liquid rises from the heated surface through the cooler bulk liquid, through free convection effects.

Remember that prior we stated that while this process took place, the bulk of the liquid is already at saturation or boiling temperature. In order for heat to enter the system, the heated wall will need to be of a higher temperature than the saturation temperature, the prior mentioned few Kelvin of superheat (superheated with respect to the saturation temperature). As the temperature field in a continuum system cannot be discontinuous, the liquid at the wall will have a higher temperature than the saturation temperature, but will still be a liquid. Some bubbles may exist on the heated wall, but they will not detach without external forcing flows.

The second phase is the nucleate boiling phase, where small vapour bubbles grow on the heated surface and detach from the surface due to the large density difference between vapour and liquid. The commencement of this phase is indicated by the ‘onset of nucleate boiling’ point, or ONB point. When the wall temperature rises above the mentioned superheat of \( \approx 5\,[\text{K}] \), small bubbles start to grow and subsequently detach from
the heated surface. This causes a higher level of mixing at the heated surface and increases the heat flux coefficient [24].

There exists a maximum heat transfer rate called the critical heat flux \( q''_{CHF} \). When the surface temperature increases beyond this point, the vapour formation rate increases so much that liquid has difficulties in reaching the heated surface. If the surface is power-controlled, this lack of liquid ‘cooling’ influx causes the temperature of the surface to rise more, leading to a destabilised system, called transition boiling, where the temperature will increase until radiative and vapour convective heat transfer is increased to a sufficiently high level, often a magnitude of superheat higher, called (vapour) film boiling. The heat transfer coefficient is lowest in the vapour-film boiling regime.

The prior introduced heat flux coefficient (see equation 2.14) can be re-computed from the heat flux values, to show that during nucleate boiling heat flux values in the order of \( 1 \times 10^4 \) [W m\(^{-2}\) K\(^{-1}\)] are reached, while the convective phase shows values an order of magnitude less.

Expressing this in Nusselt numbers would indicate a 10-fold increase in Nusselt numbers for macroscopic nucleate boiling.

### 2.3.2. Flow boiling

During flow boiling, the general idea of pool boiling holds, though now the new ‘cooling’ liquid influx to the heated surface is not just driven by density differences but also by the externally forced flow. Flow patterns seen in macroscopic flow boiling systems are shown in figure 2.5.

Two important parameters for macroscopic flow boiling are the mass fraction and void fraction, relating to the ratio of mass already evaporated of the total mass, and the ratio of volume occupied by either mass or vapour, respectively.

Of the two, the mass fraction is often easiest to calculate. Though individual portions of the fluid are hard to weigh (with \( m_V \) the vapour mass, and \( m_L \) the liquid mass), the mass fraction can also be assessed as a function of the enthalpy increase above the enthalpy of the liquid state [24]:

\[
x_{vf} = \frac{m_V}{m_V + m_L}
\]  

(2.38)

In models it is however relatively easy to keep track of the fluid enthalpy, as in equation 2.39, which results in the same mass fraction as calculated using equation 2.38:
Here \( e_L \) indicates the enthalpy for a saturated liquid, while \( e_{\text{Total}} \) indicates the enthalpy present in the fluid, and \( e_{\text{LH}} \) is the latent heat: the extra heat energy that needs to be added to a kilogram of liquid to break the bonds of the surface tension present in liquid and allow the fluid molecules to move with nearly no effect on neighbouring molecules. The latter phase is of course the gas phase.

Note that in equation (2.39) vapour superheat is not accounted for. Previously in section 2.3.1 we showed that even in macroscopic models liquid superheat can exist. As a result, if a portion of the vapour is superheated (ergo heated to temperatures above the saturation (boiling) temperature), energy is spent that is computed as if it has been used to evaporate liquid. Consequently, a mass fraction of unity, or even more than unity, calculated using the latter portion of equation (2.39), may still hold small amounts of liquid.

Next to the mass fraction, the void fraction is an important parameter in the determination of the flow properties: it represents the portion of a cross section occupied by vapour (void), shown in equation (2.40).

\[

v_{vf} = \frac{1}{1 + \left( \frac{1-x_{vf}}{x_{vf}} \right) \rho_v \rho_L S}

\]

(2.40)

Similar to the mass fraction, the void fraction can be used to determine the properties of a mixed fluid: in the case where the exact interface position between liquid and vapour phase regions is insignificant, local fluid properties may be assessed as the average properties of liquid and vapour, weighted by their volume ratio. In equation (2.40) the factor \( S \) refers to the slip ratio: often vapour and liquid no longer move at the same speed, and this effect can be captured using this parameter. The difference is often estimated based on the present flow pattern. This thesis will assume a slip ratio of 1.

Note that the void fraction can attain values close to unity for modest vapour mass fractions, as is visible in figure 2.6. Due to the high density ratio \( \approx 1000 \) between liquid and vapour, the majority of the cross section is very quickly filled with vapour, even at low mass fraction numbers. To assess the average properties in a cross-section of a fluid flow in a a duct (1D flow), the void-fraction is most often used.

### 2.3.3. Macro flow-boiling models

As introduced in the prior section, the averaged properties can be calculated using the void fraction and mass fraction of the fluid, and properties of the saturated vapour and liquid phases. As the system size is large compared to the individual bubble sizes, knowledge of exact interface location is not necessary, and as such properties can indeed be averaged.

As stated for pool boiling, the nucleate boiling regime allows for a similar increase in heat flux coefficient: more heat is transported away from the hot surface to the fluid passing. To predict this increase in heat flux, flow boiling models have been created. This is usually done by using a power law addition of two heat transfer coefficients, as in equation (2.41), where \( h_{\text{nfb}} \) is denoted as the nucleate boiling heat transfer coefficient, and \( h_{\text{cfb}} \) as the convective flow boiling heat transfer coefficient [25]. The former is most influenced by the
temperature difference between the heated surface and the mean flow temperature, while the latter is most dependent on the Reynolds number, and as such on the flow velocity [24].

$$h_{fb} = [(h_{nfb})^n + (h_{cfb})^n]^{1/n}$$ (2.41)

These boiling heat transfer coefficients are often determined using an empirical basis, and are usually limited to a certain set of flow conditions, but more importantly to a maximum vapour mass fraction. Creating consistent heat transfer models for the full evaporation range (from a 0 vapour mass fraction to unity) is not often undertaken, as during the higher void-fraction levels, the heat absorbing qualities of the fluid decrease, and the often used goal of maximum cooling of the surface is not attained.

Furthermore, as mentioned these models focus on maximum cooling rates, and are often set up for turbulent flows. As these macro-scale models are no longer applicable for very small channels [18, 24], they will not be expanded upon.

2.3.4. DISCERNING MACRO-SCALE BOILING FROM MICRO-SCALE BOILING

Macroscopic flow-boiling models introduced above rely on the ability to average out fluid properties based on the ratio of the phases in a volume or cross section. Accurate interface positions are therefore not required.

However, micro-scale systems behave profoundly different: due to the limited volume present in small systems, a small amount of vapour generated will quickly envelop a relatively large volume in the flow system. For instance, in the currently investigate VLM design, the height dimension is very small. When a liquid volume cube with rib lengths of $1 \times 10^{-3}$ of the height of the heater is evaporated, the density ratio of liquid to vapour of approximately $1 \times 10^3$ dictates that this element now expands to encompass the full height of the system, and simultaneously push liquid away in both lengthwise and width directions.

This example shows that the resultant fluid domain is occupied by alternatively a pure liquid, or a pure vapour. As such, mass fraction terms would read either 0 or unity, with a very thin border separating the two phases where some degree of mixing of phase occurs [26].

Micro-scale models need a different approach compared to the property-averaging macroscopic approach. The first thing is then to identify the cases of micro-scale flows. The distinction is best made using either the Bond number or its square root inverse, the Confinement number:
2.4. MICROSCOPIC TWO-PHASE EVAPORATIVE FLOW

Both indicate the ratio of the body force difference on each phase based on gravitational acceleration versus the surface tension forces. We can calculate the Bond number using approximate values for density difference \( \Delta \rho = 1 \times 10^3 \) [kg m\(^{-3}\)], gravity acceleration of \( g_0 = 9.81 \) [m s\(^{-2}\)], Hydraulic diameter of \( D_h = 0.29 \) [mm] and surface tension of approximately \( \sigma = 60 \) [mN m\(^{-1}\)] (see appendix D), to find a Bond number of 0.0138, where numbers less than unity are considered indicative of micro-flows [24]. Ergo, the surface tension effects dominate the fluid flow at these hydraulic diameters, and using average fluid properties oversimplifies the boiling system.

As indicated in section 2.3.4, the current VLM design can clearly be identified as a micro-flow-boiling system. As such, the behaviour of micro-flow-boiling systems, as well as currently employed modelling efforts will be discussed in this section.

One of the key elements that was used in the prior section to differentiate macroscopic from microscopic evaporative flows is the surface tension coefficient \( \sigma \). This of course refers to the effect of surface tension. [17] suggests that surface tension can be understood to be the net attraction forces that liquid molecules experience from their neighbours that are present, and the lack of attraction forces where the vapour region starts. Consequently, the interface surface of the liquid is in tension. The net effect is calculated as a pressure jump across an interface, using equation 2.43:

\[
\Delta p = \sigma \left( R_1^{-1} + R_2^{-1} \right)
\]

Here \( R_1^{-1} \) and \( R_2^{-1} \) represent the two curvatures present. For a spherical bubble, the two curvatures are the same, and the pressure jump reduces to Young-Laplace relation [27]:

\[
\Delta p = \frac{2\sigma}{R}
\]

2.4.1. MICRO-FLOW-BOILING BEHAVIOUR

According to [28], who investigated flow boiling instabilities in micro-channels, there exist two main categories of instabilities: classic instabilities, indicating a shift of operating point (flow excursion (Ledinegg instabilities), boiling crisis and flow pattern transition), or dynamic instabilities, indicating oscillatory flow behaviour around a steady operating point (density-wave oscillations).

In the study of mechanisms and control, unstable systems are defined as systems that will deviate from the initial conditions with increasingly large magnitudes (unbounded growth) given a perturbation of one or more of the states. However, in the study of micro-flow-systems, this definition is muddled to two new types of instability:

The ‘static instability’ is an essential type of instability to assess, as it can drastically change system behaviour (as such, this lines up with the classical definition of an instability), while the ‘dynamic instability’ refers to oscillatory behaviour that can be neglected if the oscillations do not reach magnitudes or frequencies that induce static instabilities. An example of a case where oscillatory behaviour is able to interrupt nominal functioning of the system, is for a VLM, where instead of pure vapour liquid droplets or even a fully liquid flow will enter the nozzle, resulting due to a lack of compressibility of the fluid in a reduced exhaust velocity, and reduction of ISP.
Some models predicting the oscillation behaviour exist, though they are very situation dependent. [28] suggests a frequency prediction model, where using fluid properties and evaporation speed a frequency assessment of the oscillations can be made. It is unfortunately only available for simple ducts (where 1D approximations are possible), and the characteristic recoil length is required information, which is unfortunately impossible to obtain in the current VLM design, due to lack of visual high-speed data in comparable designs to the current VLM design.

**Observed behaviour**

Large pressure fluctuations are noted by [29] in parallel channel systems due to flow-recoils when expanding bubbles pushed the liquid-vapour interface in both upstream and downstream direction. Smaller oscillations are seen in the parallel heat channels, and correlated with intermittent flow speed exchange between parallel channels.

Similar fluid flow and at times periodic oscillations are observed by [30]. These tests, alike those shown by Kandlikar are all however performed for Reynolds numbers of 100 and up, or for mass fluxes upwards of $120 \text{ kg m}^{-2} \text{s}^{-1}$.

Slow flow oscillations ($< 1 \text{ Hz}$) are observed by [16], and according to the author attributed to compressibility of both the vapour and the feed system, while faster oscillations ($> 1 \text{ Hz}$) are similarly observed, and are suspected to be density-wave oscillations.

[31] goes as far as stating that two-phase evaporative flows in micro-thrusters are always unstable. They investigated the coupling between feed pressures and recorded thrust values for a VLM model, showing that these are indeed very closely linked. As such the observed fluid flow (velocity) oscillations and pressure oscillations describe all but the same phenomenon, and given the very small amount of mass in micro-systems in the system, it is not surprising to learn that velocity and pressure oscillations are closely coupled. Figure 2.7 shows the force versus pressure coupling: with every increase in pressure, a simultaneous increase in nozzle force is recorded.

Given the equations 2.34 and 2.37, any increase in chamber pressure will result in an increase in mass flow rate through the nozzle, and a subsequent increase in force actuated by the VLM. [31] observed pressure fluctuations range from near 0 to 47[kPa], while periods of oscillations are said to vary from 'short' (< 0.5[s]) to $\approx 4.3$[s].

Rops [24] cites among others Tadrist to indicate the large fluctuations in pressure for single-duct micro-boiling heaters. Especially given constant pressure inlet conditions, pressure fluctuations in excess of 30[kPa] were recorded, as is seen in figure 2.8. Note that these fluctuations quickly decrease with increasing Reynolds numbers, and no longer seem to occur at all in the turbulent regime.
Zhang et al [32] discovered even larger pressure fluctuations in single-duct micro-flow-boiling systems, with local pressures of up to 138[kPa], where systems exited to ambient pressure, ergo locally increasing the pressure to over double that of the exit pressure. They further noted that depending on both surface roughness and wall temperature either a more nucleate-like flow-boiling behaviour (larger surface roughness capable of hosting a large amount of vapour nuclei) leading to annular flow or eruptive boiling (both higher wall temperatures and smoother surfaces) took place.

Finally [16] suggest that in wider systems, where 1D duct flow seems to be too much of a simplification, in cases of insufficient power influx, a snake-flow pattern can arise (see figure 2.9). Note that the flow pattern shows approximately the same cross-section for the liquid in the wide heater section, as the width of the inlet section, and continues down the heater. The path of the flow was observed to oscillate.

**HEAT TRANSFER BEHAVIOUR**

Kandlikar [29] notes the observation of bubbly, slug and annular/slug flow, and annular/slug flow with nucleate boiling dry-out, for hydraulic diameters in the order of 1[mm]. However sustained dry-out, meaning complete evaporation in a section of the system, is unattainable for superheat temperatures of 20[K].

Zhang [32] discovered that increasing surface roughness can promote nucleation sites for nucleate boiling, and as such reduce the chance on explosive or eruptive boiling in small channels. However, the studies have been conducted only for superheats up to about 20[K], and higher wall superheats seem to indicate a near unavoidable explosive boiling behaviour.

Concerning the occurrence of bubble explosions: [31] report that these occur most predominantly at sharp flow-interruptions such as the inlet section of the 9 smaller channels seen in their experimental set-up.

**SUMMARISING MICRO-FLOW-BOILING BEHAVIOUR**

Concluding, micro-flow-boiling systems are prone to both oscillatory and at times unstable behaviour, with very large transient pressure pulses due to what is dubbed ‘explosive’ or ‘eruptive’ boiling. Due to the small dimensions, local pressure peaks significantly perturb the flow as observed by the oscillating force measurements. Zhang et al measured 138[kPa], is it possible that higher pressures also occur, and what effect does this have on the system design? This focus on instability is in sharp contrast to the behaviour of macroscopic boiling systems, where predictable behaviour seems to be key.
2.4.2. **Behaviour Specific to VLM’s**

Though a VLM implicates a ‘vaporising liquid micro-thruster’, the ‘vaporisation’ part is not to be taken for granted. As suggested by [16], four distinct flow patterns through the nozzle structures and exiting the VLM are observable:

1. Snake-flow, or liquid flow, indicating the complete lack of significant evaporation and liquid flowing through the nozzle, lacking any kind of acceleration in the nozzle structure, as seen in figure 2.9.

2. Vapour-droplet flow, where the liquid path was broken up by evaporation, but still a significant portion of the excreted fluid was in the liquid phase, consequently lacking significant acceleration through the nozzle.

3. Vapour-droplet jet-flow, where the larger portion of the volume is occupied by vapour, but a significant amount of dispersed liquid droplets remain in the VLM, and by virtue of the accelerating vapour through the nozzle the liquid droplets get dragged along, and are ejected with some force.

4. Vapour flow, the desired outflow mechanism, where all liquid is evaporated before reaching the nozzle, and consequently is able to attain it’s maximum acceleration potential and maximum specific impulse.

The term spitting, as suggested by experts in the field of vaporising liquid micro-thrusters, refers to incomplete evaporation of the propellant, either flow pattern 2 or 3. Remarked in the work of [8], spitting can cause a drastic reduction in propellant efficiency, and all effort possible should be spent on preventing this phenomenon.

However, the inherent oscillatory behaviour of micro-flow-boiling systems, as described in section 2.4.1, can cause a seemingly sufficiently heated system to still eject liquid droplets intermittently.

To increase the understanding of the spitting phenomenon, the Saffman force [33] is perhaps an interesting path of further investigation, relating how spherical particles, such as liquid droplets, are attracted to the centre of a faster moving viscous flow. An understanding of these forces and their relation to spitting might enable design improvements that maximise the odds of liquid droplets impacting with heated surfaces and subsequent evaporation occurring. However, this study lies outside the scope of this thesis.

2.4.3. **Current micro-flow-boiling models**

As concluded in both the previous sections and by [18], macro and micro boiling are vastly different when attempting to model the system. The current state-of-art of micro-flow-boiling models focusses on one of the main envisioned usages for such systems: the cooling of high-powered computers. As such, the heat flux coefficient drop for higher vapour qualities make using the complete evaporation range impractical.

However as [18] suggests, during the initial micro-channel boiling very high heat fluxes in excess of $6 \times 10^4$ [Wm$^{-2}$K$^{-1}$] [34] are noted for micro-channels with a hydraulic diameter ranging from $1 \times 10^{-2}$ to $1$ [mm].

Such very high heat fluxes might induce temperature gradients in the base structure, that might in turn be disruptive to fluid behaviour, or might even damage structures, and as such should be investigated.

Heat correlation models for high mass flux systems ($> 200$[kgm$^{-2}$s$^{-1}$]) have been near-simultaneously developed by [34] and [25], the former based on annular flow systems, the latter based on slug flow with wetted walls. [34] shows the model ranging from a vapour quality of near-zero to 0.2, while [25] seems to show the model for vapour qualities of up to approximately 0.15.

However Qu [35] noted that most of the present correlations were unable to accurately predict heat transfer, even the correlations created for mini/micro channels. Moreover [35] notes that the saturated flow boiling heat transfer coefficient is more strongly a function of mass flow than of heat flux, suggesting that the method of heat transfer is more due to convective than boiling transfer.

The latter conclusion is of importance to the present study, as the mass fluxes reported by [25, 35–37] when mentioned lie in the region upwards of 100[kgm$^{-2}$s$^{-1}$], while the present research focusses on modelling a mass flux of approximately 2[kgm$^{-2}$s$^{-1}$]. As such, the conclusion of [35] predict bad correlations between existing higher-mass flux correlations and the intended low mass flux VLM application. The mass flux is a measure for mass per cross-sectional area, [kgm$^{-2}$s$^{-1}$].
\[ G = \frac{\dot{m}}{\lambda_{cs}} \]  

Finally, as indicated by the models presented by from [25, 34, 35], the models created currently focus on only partial evaporation, as during full evaporation the heat flux coefficients drop markedly when the vapour mass fraction increases [18]. This investigation of the critical heat flux is also assessed as one of the key future study subjects by [36]. As the goal of the VLM is to model the full evaporation range present in the thruster, this poses a challenge.

2.5. VLM DESIGNS AND MODELLING

While the above mentioned boiling behaviour and existing modelling attempts are mainly focussed on cooling systems (with the exception of section 2.4.2), it is essential to study existing VLM designs to be able to judge the expected performance of the TU Delft VLM. Furthermore, knowledge of applied models in currently published VLM designs might provide extra insights into the modelling that will be attempted in this thesis.

For further information on the designs lay-outs of, see appendix A.

2.5.1. CURRENT DESIGNS

Out of plane thrusters have been presented among others by [13] and [38], where the former worked by continuously feeding water through, and the latter used a pulsed-firing method. Out-of-plane refers to the method of production, where important design features such as the nozzle are formed mainly using anisotropic etching techniques, generating structures that vary in the height-direction. Both designs presented were able to attain similar \( I_{sp} \) values of \( \approx 75 [s] \), using a 3D nozzle structure by etching along the naturally created etch surfaces of Silicon to form a pyramidal nozzle of fixed expansion angles. They note that unfortunately these angles are too wide to allow for efficient fluid accelerations.

In contrast, [15, 16, 31, 39] showcased VLM’s with in-plane essentially 2D nozzles. The specific impulse values attained by Cen and Kundu ranged up to \( \approx 105 [s] \). It appears that though these planar systems are restricted in the possibility for nozzle shapes, more fitting 2D convergent and divergent angles can be chosen, in contrast to the fixed angles in the out-of-plane nozzles, resulting in relatively high specific impulses. Furthermore, research at Dimes (the TU-Delft MEMS and silicon lab) is ongoing to create viable methods for 3D shaped systems, which could be extended to 3D ’in-plane’ nozzles, allowing full freedom on the choice of angles.

Notably, [39] chose a different production method compared to other presented VLM’s: instead of opting for a silicon base structure, they chose a structure built with ‘high-temperature co-fired ceramics’. The advantage is a markedly lower thermal conductivity of the ceramic structure compared to the silicon base structure, possibly boosting efficiency by reducing heat-losses. Unfortunately the ceramic structure is prone to breaking as cool liquid hits the heated surface, and as a result is a poor choice due to these reliability issues. Furthermore, [15] have reported similar efficiency values for their thruster, though their mounting system is unclear.

Rob Poyck and Ivan Krusharev [10, 11] provided designs attempting to improve the efficiency levels of the VLM heaters using a silicon base structure, but with the heaters suspended in the liquid flow. Furthermore, a scalable architecture was envisioned, so the basic VLM design can be easily adjusted to new mission demands specifying changes in pressures or temperatures. The new design attempts to use heat-flux enhancing elements, such as the pillars introduced in figure 2.2. Different other models, including winding channels, have also been proposed. Parallel duct systems have previously been shown to function by [31]. However given the thin-film like system, it appears that it is not necessary, according to the study performed by [16], as they show successful complete evaporation without the use of duct-systems or pillars.

2.5.2. CURRENT MODELLING EMPLOYED

In most of the the presented VLM publications, limited information is provided on modelling. Some such as [10, 15] model the nozzle flow with single-phase CFD calculations, while [13, 14] show analytical models to calculate the expected efficiencies. These latter models are especially useful, as they allow the designer to quickly evaluate their design.
However, the models by [13, 14] present no knowledge on the required power distribution in the heating chamber, nor do they provide useful estimates on matters such as residence time: though both calculate a value, this is based on the liquid density, and is therefore over-estimated.

None of the uncovered VLM publications have shown two-phase fluid-flow modelling. As a consequence, none of the available design methods are able to judge the systems likelihood of showing spitting behaviour (see section 2.4.2).

2.6. CHAPTER SUMMARY

This chapter has provided a wide overview of knowledge and theory required to grasp the tackled elements in this thesis. This ranged from fluid mechanics and heat transfer, to isentropic nozzle flow equations, and on to both macroscopic and microscopic boiling phenomena. Unfortunately it must be concluded that no sufficient modelling approaches are available to predict system behaviour for a VLM as designed by the TU Delft.

Two modelling strategies can be investigated as viable approaches:

1. Simplified heat flux modelling, where a 1D model is set up, based on a simplified flow pattern analysis. This model can be used to judge desired system temperatures and heater power. It will have to be correlated to a fully-evaporative low-mass-flux system, to ensure reasonable accuracy.

2. Attempt to model the full system behaviour using fundamental flow equations such as the Navier-Stokes equation, or a first-principle approach, and using a finite-volume-element model of the design domain to allow for both static as well as dynamic oscillations. Such a model would in all likelihood offer the greatest insight into design optimisations, and if the computation costs can be sufficiently reduced, might offer opportunities for a full-domain numerical optimisation.

Approaches for both methods will be introduced in the next chapter.
Analytical models

Initially this chapter will present short investigations on some questions raised by the combination of suspended wire heaters, the large difference in the heat conductivity of the fluid versus the base silicon material, and the explosive boiling phenomenon observed by [32], and previously explained in chapter 2. Specifically section 3.1 will detail the expected path of heat transfer, from wire to fluid, while section 3.2 will investigate the mechanical considerations in using thin heating wires. Section 3.3 will investigate an option to restrict reverse flows due to large pressure fluctuations while evaporating.

Next three separate models will be presented in this chapter. First the energy-balance model (or just balance model for short) will be introduced in section 3.4, and will be used to identify specific impulse values that can be theoretically attained, and to assess efficiencies of the system, an investigation so far not yet performed. It will be used to judge if the mounting methods are sufficiently isolating given the limited power budget, and given the blow-down mode of operation, what thrust levels can be expected throughout the mission life, as well as when the maximum power requirements will be demanded from the heater system.

The second model is the steady-state 1D fluid flow model presented in section 3.5. It provides information on the expected fluid temperature distribution in the heater, as well as information on the required sustained silicon wall temperature of the heater to ensure full evaporation. The publications [16] and [31] will be used to correlate the heat-flux for the two-phase regime to experimental data, to attain improved model accuracy. More details on the publications and the way the data is used to correlate models is available in appendix B.

With the known average power distribution calculated using the 1D model, and a uniform power influx, a measure for the temperature gradients occurring in the silicon base structure is calculated, to investigate if large gradients will occur, or if the uniform-temperature assumption will hold.

In section 3.6 a time-dependant 1D model is introduced, to assess minimal wall temperatures needed during start-up behaviour, and if start-up conditions (with near-vacuum pre-existing pressures in the heater chamber) require extra design constraints.

Section 3.7 highlights what questions are answered, and which are still relevant and unanswered.

3.1. Methods of heat transfer

Earlier in chapters 2 the layout of the thruster design by [11] was simplified by discounting the diamond-shaped pillars. This simplification is posed to reduce the complexity of the heat transfer calculations. As these pillars are expected to enhance heat transfer, this simplification suggests a worst-case scenario test and as such is an acceptable simplification.

Work performed by [40] shows that for low-Reynolds numbers (Re< 100) diamond pillars added to the flow of a single-phase micro-system double the Nusselt number observed for a plain micro-channel. Consequently the plain-case is expected to have a Nusselt number of 6.0 based on the tables reported by [18], while the case involving dispersed diamond pillars is expected to show an increased Nusselt number of at least 12.0, as the work performed by [40] introduced pillars prior to the heated area, and therefore relayed only on the
persistence of the flow disruptions continuing into the heated area, while the design by [11] introduces pillars throughout the heated section, ensuring that flow-disruptions will keep occurring.

### 3.1.1. **DIRECT WIRE TO FLUID HEATING**

The design by Poyck [11] is based on 'floating' heating wires crossing the distance between its suspension points at pillars or other structures, as seen in figure 3.1. Note that this image can be taken from any section of the main body of the heater, section 2 of figure 2.1a.

![Figure 3.1: A drawing from a small section of the heater: the silicon base structure with the thin and small silicon-carbide heating-wires resting on top of the silicon pillars (not to scale).](image)

Poyck hypothesised that by suspending the heaters, losses through the silicon structure to the satellite frame could be minimized [11]. This relies on two assumptions:

1. Heat transfer from wires directly to the fluid is very efficient
2. Consequently, the heat transfer through the wires into the silicon pillars, and consequently into the silicon base structure is so slim that the outer system walls are at a significantly lower temperature than both the fluid and the wires.

The second assumption is in fact a curious one: if the fluid is assumed to be (nearly) uniformly heated to the desired final temperature, this entails that fluid at the walls of silicon is raised to close to this temperature. The very high silicon conductivity, when compared to the vapour conductivity (149[Wm$^{-1}$K$^{-1}$] vs. $\approx0.03$[Wm$^{-1}$K$^{-1}$]) then ensures that any heat flowing from vapour to silicon wall will very quickly be distributed throughout the silicon base structure. This leads to one possible outcome:

Vapour near the silicon wall experiences significantly lower temperature than vapour in the centre of the flow, reducing the propellant efficiency (see equation 2.30, 2.34, 2.37 and 2.17).

The following computations will test whether this assumption is correct.

### 3.1.2. **WIRE THROUGH SILICON TO FLUID HEATING**

The conclusions of the previous section, depend on the primary assumption that the heating wire is exceedingly efficient in losing its heat to the fluid. However, when for instance the surface ratio of wire-surface compared to available silicon surface is computed, a very small ratio is uncovered:

$$A_{\text{ratio}} = \frac{A_{\text{wire}}}{A_{\text{Si}}} \approx 0.0015 \quad (3.1)$$

Here the silicon structure area is computed as the summation of the silicon floor length and the area of the silicon pillar, with dimensions used as designed [8] (see appendix A).

This very small ratio indicates that the fluid passing has very little opportunity to come into contact with the heating wire. If it does, the relatively low fluid conductivity will require a significant temperature gradient to ensure a high power flux through such a small area surrounding the wires.
If however it is assumed that the no heat is 'lost' from the wire to the liquid, and all the heat generated in the wire is transported to the pillar, where it is redistributed throughout the silicon, the temperature drop over the wire can be computed.

Given the $Q_{\text{section}} = 1[W]$ of power distributed over 8 rows of 50 'suspension-and-free-hanging-sections' (the repeated module), the heating power per repeated module is approximately $Q_{\text{module}} = 2.5[mW]$. Based on the shorter length but smaller width of the free-hanging section, approximately half this power will be generated in the free-hanging section. Applying equation 3.2, and using as indicated half the suspended length ($L/2 = 10[\mu m]$) and the reported heater width and thickness ($W = 9[\mu m], t = 300 [nm], A_{\text{wire}} = W \cdot t$), with the heat conductivity of silicon carbide $\kappa_{\text{SiC}} = 490[Wm^{-1}K^{-1}]$, the maximum temperature difference is computed to be only 9.8[K].

$$\Delta T_1 = \frac{Q_{\text{module}}}{2} \frac{L/2}{\kappa_{\text{SiC}} A_{\text{wire}}}$$  \hfill (3.2)

A similar approach is used to calculate the temperature drop in to the pillar base area. The base of the pillar is approximately half it's length multiplied by the width ($L = 160[\mu m], W = 40[\mu m]$), while $H = 75[\mu m]$ represents the height of the pillar.

$$\Delta T_2 = Q_{\text{module}} \frac{H}{\kappa_{\text{Si}} A_{\text{pillar}}}$$  \hfill (3.3)

This results in an approximate temperature gradient from the pillar to the silicon base of $\Delta T_2 \approx 4[K]$. That includes the thin silicon oxide insulating layer positioned between silicon carbide and silicon base structure. Of note is that the current batch of heaters has been over-etched, reducing the area of the pillars, and increasing the temperature gradient to approximately $\Delta T_2 \approx 16[K]$, though this pillar is already in contact with the fluid over a substantial area.

The very much larger surface area available for silicon-fluid interactions lends credence to the theory that most heat will be conducted through the silicon structure to the fluid. Therefore the added 'isolating' effect of having floating heating wires appears to be minimal.

Next to the design with small pillars, [8] has proposed also designs with larger pillars and wider overhangs for the heating wire. These designs show a very large temperature gradient of approximately $\Delta T_1 \approx 167[K]$ over the full span. Due to the very small surface area and subsequent difficulty of releasing heat to the fluid, this system might provide some issues. Such a mismatch in temperature of the wire might lead to a relative expansion of the wires compared to the structure, inducing extra stresses in the wires.

This thesis will focus on the small-diamond model.

### 3.2. Fragility of heating wires

The heating wires are furthermore reviewed based on robustness of their design. In chapter 2 data gathered by Zhang et al. [32] was presented that indicated very high transient pressure pulses on heated surfaces, for only modest superheat temperatures. Given the goal of having superheat temperatures of an extra magnitude (100[K] instead of 10[K] used by [32]), the measured pulses of 1.38 [bar] seem to be on the low side. This pressure loading would most likely occur at the hottest point of the solid surface first, resulting in a pressure pulse in the middle of the suspended heater.

Examining a worst-case scenario, where the full width of the wire is subject to a pulse of 1.4[bar], or $1.4 \cdot 10^5[Pa]$, this relates to a distributed force over the full length of the wire. The force per unit length on the wire is expressed as:

$$F_{\text{dist}} = p_{\text{pulse}} W_{\text{wire}}$$  \hfill (3.4)

This force $F_{\text{dist}}$ is subsequently multiplied by its distance to the mounting point, and integrated over the length to obtain the contribution to the moment at the mounting point.
\[ M_{mp} = \int_0^{L/2} (xF_{\text{dist}}) \, dx \quad (3.5) \]

This results in a maximum moment at the mounting point of approximately \(6.3 \cdot 10^{-11} \text{[Nm]}\). Using equation 3.7, the maximum stress (both tensile and compressive) is calculated. In the large rhombi case, with a total overhang length of \(L = 180 \times 10^{-6} \text{[m]}\), the maximum moment is \(2.2 \cdot 10^{-8} \text{[Nm]}\).

Next, the second moment of inertia is calculated for both cases.

\[ I_x = \frac{Wt^3}{12} \quad (3.6) \]

The bending stresses are calculated next:

\[ \sigma_{\text{bending}} = \frac{Mt/2}{I_x} \quad (3.7) \]

Shear stresses are similarly accounted, and the maximum is assessed by assuming a parabolic shear stress distribution:

\[ \sigma_{\text{shear}} = \frac{3 F_{\text{dist}} L}{2 W \cdot t} \quad (3.8) \]

The bending stress for the small rhombi case peaks at 466.67 \text{[MPa]}, while the shear stress peaks at 7 \text{[MPa]}. Mono-crystalline silicon is observed to be able to cope with much higher stresses at times, however stress concentrations due to manufacturing, have seen silicon structures break without any apparent reason [41]. As such, allowing for such high stresses in the structure seems ill-advised. Taking into account that the experienced stresses might be exacerbated by the possible already present compressive stresses due to the non-uniform heating, a redesign might be appropriate.

Again, note that, 8 rows holding, 100 separate possible fracture points, are mounted per heater section, and 7 of these sections are intended to make up the heater section of a single heater. Consequently, this design provides 5600 (!) individual failure points.

A single failure will be able to destabilise the rest of the section, as 8 rows are connected to a single current-controller, and the remaining 7 intact heater wires are now subjected to an increased current density, and consequently will be heated to higher temperatures, resulting in more stress due to the expansion of the wires, and possibly more violent evaporation explosions due to the higher temperature.

The large rhombi case will most likely lead to immediate failure, as the bending stresses peak at 37800 \text{[MPa]}, while shear stresses amount to 63 \text{[MPa]}. It is therefore strongly advised not to use the large-rhombi cases with evaporating fluids.

### 3.3. Reverse-flow restrictions

Given the pressure pulses and large reverse-flows observed by among others [24, 25, 29, 31, 35], pulses in the order of 0.5 \text{[bar]} are expected to be common occurrence, and might result in oscillatory flow patterns. Such oscillatory flows are unwanted, as they impede predictable operating behaviour, or might even lead to sputtering of the thruster despite a steady-state sufficient power influx. Therefore reducing the oscillations produced during evaporation in the thruster is an avenue worth investigating. Flow restrictors, placed upstream of the heater, might be a useful design addition. These have been employed by [39] in their VLM design.

However, as the pressure oscillations are potentially very large, significant pressure would have to be lost over the restriction, resulting in a loss of performance of the system due to the blow-down mode of operation (no means of compensating for lost pressure).

To accommodate this, a one-directional valve would provide a sufficient solution. Moving components are however expected to reduce system reliability, and given the troubles in attaining reliability of moving parts in a MEMS systems of similar dimensions as the heater, a valve without moving parts is called for. Perhaps a design based on the patent [42] is applicable, adding a modest pressure drop in ‘free-flow’ direction, and a significant (according to patent order of 200 times larger) pressure drop in reverse flow, or ‘obstructed-flow’
direction. The working principle of the ‘valvular conduit’ is shown in figure 3.2, with in green arrow indicating the free-flow direction, while in red the high-pressure-drop obstructed-flow paths are shown.

As the fluid flows into the obstructed-path direction (right to left), fluid has the tendency to follow the smooth wall surface, resulting in repeated flow-excursions in channels that reverse in direction, and the fluid flowing through this section is used to hinder and slow the fluid flowing in the main zig-zag path, effectively increasing the pressure drop over the section for the same fluid velocity. This effect only becomes significant in flows where the inertia effects are not negligible. According to [43], inertial effects only become noticeable around Reynolds numbers of $1 \times 10^2$, so the use of the shown valvular conduit should be investigated thoroughly before applying it to the system.

Figure 3.2: The ‘valvular conduit’, by N. Tesla, adapted from [42]

The green path indicates the low-pressure inducing path (left to right), with the off-centre paths barely contributing to the flow or providing hardly any obstruction. Some investigations into the application of such valves in micro-fluidics have been conducted by [44], while [45] investigated topology optimisation of similar valves in micro-fluidics for single-phase fluid flow.

3.4. ENERGY-BALANCE MODEL

The energy balance model is a very versatile and relatively simple model. No assumptions are made concerning the fluid flow, residence time or pressure drops over the heater. Instead, using the IRT calculations (see section 2.2) mass flows are estimated based on inlet pressures and vapour temperatures. Consequently the power drawn by the fluid to sustain the mass flow rate and the final temperature are calculated, and added to calculations relating to expected heat losses. This results in both values for the performance, and efficiency. So far [8] included investigations on the expected mass flow through the nozzle and the power required to heat the liquid to desired temperatures at the estimated mass flow rates, but no efficiency calculations were performed (50% efficiency was assumed), and no expected specific impulse values are reported.

The heat-balance and efficiency calculations of similar nature have been reported on by [13, 14].

The balance model is split up in 4 main domains:

1. Calculate the expected mass flow at a desired wall temperature and pressure
2. Calculate the needed power to heat the fluid up to the wall temperature at the feed-pressure
3. Calculate the conductive and radiative losses to the environment
4. Finally calculate the thermal efficiencies and ISP values.

These calculations will be executed on the general dimensions of the system by [8], as presented in appendix A

3.4.1. MASS FLOW RATE CALCULATION

The first component to be calculated is the mass transported through the system. To do this, equation 2.34 is applied. The desired wall temperatures are varied with steps of 20[K]. Similarly, pressures that are tested with steps of 1.0[bar] per iteration.

<table>
<thead>
<tr>
<th>Element</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_c$</td>
<td>430 – 670[K]</td>
</tr>
<tr>
<td>$T_{in}$</td>
<td>293[K]</td>
</tr>
<tr>
<td>$p$</td>
<td>0.5 – 5.5[bar]</td>
</tr>
<tr>
<td>$C_d$</td>
<td>0.7</td>
</tr>
</tbody>
</table>

Table 3.1: Test criteria set
Throat dimensions are used as measured from the produced thrusters [8], see appendix A. For the algorithm, please see the appendix H.

![Figure 3.3: Mass flow calculation using the IRT](image1)

The resultant mass flow rates are plotted in figure 3.3, showing the mass flow rate for some of the tested pressures, over the full temperature range. Observable is that the mass flow rate increases linearly with pressure, though it decreases slightly with increasing temperature. This can be explained using equation 2.34, repeated here for convenience:

\[
\dot{m} = C_d \frac{p_c A_1 \Gamma}{\sqrt{k T_c}}
\]

An increase in pressure relates indeed linearly to an increase in mass flow, while the mass flow decreases with the square root of the temperature.

### 3.4.2. Fluid Power Requirements

Using the XSteam program [46], which in turn uses tables based on the 'IAPWS IF-97' standard [47, 48], saturation temperatures and at the tested pressures are determined. Next, the energy required to heat the fluid is determined by the difference of enthalpy in the liquid at inflow temperatures, with the enthalpy of the vapour at the desired final temperature.

\[
\Delta e = e_2(T_c, p) - e_1(T_{in}, p)
\]  

(3.9)

In equation 3.9 the \(T_c\) or chamber temperature refers to the desired final temperature of the fluid, while \(T_{in}\) refers to the fluid inflow temperature, and sub-indices 1 and 2 refer to the initial condition and the final condition, respectively.

Next the power required to heat the fluid is determined based on the mass flow rate (as calculated in equation 2.34) and the calculated energy value (as in equation 3.10).

\[
P_h = \dot{m} \Delta e
\]  

(3.10)

The results are shown in figure 3.4. Note that for higher temperatures at the same pressure, marginally less power is required to heat the fluid. This might be counter-intuitive, as the energy required to heat a unit of mass of vapour to a higher temperature obviously increases. However, as seen in equation 2.34, the expected mass flow decreases with \(T^{-1/2}\), and as such the net power required decreases. Considering the latent heat as
3.4. ENERGY-BALANCE MODEL

Figure 3.4: Power needed to heat the fluid to the wall temperature, at the inflow pressures.

the major specific energy ‘sink’ in the fluid-heating process, it is understandable that the limited extra energy needed for an increase in temperature is offset by the mass rate reduction.

For instance, the specific energy increase for the 5.5 [bar] case, when increasing temperatures from 450 [K] to 650 [K] can be computed using equation 3.9, where instead of the inflow temperature $T_{in}$, the lower chamber temperature of 450 [K] is set, and as $T_c$ the upper temperature of 650 [K] is set. The result is a difference of $4.2 \times 10^5$ [J kg$^{-1}$], on a total specific energy for the 450[K] case of $2.8 \times 10^6$ [J kg$^{-1}$], representing an increase of 15%, while the mass flow calculated using equation 2.34 decreases with 20.1% between the 450[K] and the 650[K] case. The net result is a reduction in total energy request, of 4.3%, or 0.15[W], between the investigated cases.

EXPECTED POWER LOSSES

Heat losses, and subsequently power losses, are expected to occur due to conduction through the supports of the thruster, and radiation from the outside thruster surface to space. Conductive heating loss due to heat leaking upstream into the fluid-supply system is discounted here, as this preheats the fluid and therefore still serves its purpose.

The conductive heating losses are determined using the assumption that the outside surface of the heater is at the same temperature as the inside wall and vapour temperature used for the calculation of the power requirements and mass flow rates. This correlates with the small temperature gradients that were discovered in section 3.1. The satellite structure temperature is assumed to lie at the liquid inflow temperature (see table 3.1). Next a one-dimensional conductive equation is used [49]. As per current design by Tiemen van Wees, the system is intended to be supported by small glass squares (see figure 3.5, with the pillars circled), having rib-lengths of $L_{support} \approx 0.5$ [mm], whose conductivity is approximately $\kappa_g \approx 1.09$ [W m$^{-1}$ K$^{-1}$] [49]. The conductive losses are computed using equation 3.11.

$$P_{cond} = \kappa_g L_{support}(T_c - T_{in})$$ (3.11)

Radiative losses are computed using a similar assumption. As a worst-case test, the full surface area of the heater is used as if it were radiating to empty space. In reality, the ‘underside’, or the side of the heater mounted using the aforementioned pillars will radiate towards the structure. As an emittance factor, aluminized exterior is assumed, with an emittance factor of $\varepsilon \approx 0.05$ [49], while the Stefan-Boltzmann constant is held at $k_{SB} = 5.670373 \cdot 10^{-8}$ [W m$^{-2}$ K$^{-4}$], as per [49]. The computation is performed using equation 3.12.

$$P_{rad} = \varepsilon k_{SB} T_c^4 A_{ext}$$ (3.12)
As both conductive and radiative losses are independent of fluid flow, but instead solely dependent on used wall and fluid temperature, their evolution with this temperature is plotted in figure 3.6.

![Figure 3.6: The power loss based on wall temperature, for both conductive as well as radiative losses.](image)

In figure 3.6 the linearly increasing conductive losses clearly have a greater power draw than the radiative losses, for the temperature range investigated (see table 3.1).

The total power requirements, comprised of both the power draw by the fluid flow (seen in figure 3.4) and the losses (seen in figure 3.6), are plotted in figure 3.7. The decreasing power-requirements for the fluid flow for higher wall temperatures, due to the reduction in mass flow, are offset by the increased expected losses. However, for all the investigated operating conditions, the power required remains well within the posed power envelop of 7 [W] (see table 1.1), as chosen when specifying the system requirements by [8].

The power usage of the thruster visible in figure 3.7 is indeed a reduction of nearly 40% compared to the figures quoted by [8]. Based on these results a reduction in system length is viable, further reducing radiation losses. However, as they only comprise about 29% of the expected losses, the gains using this method are limited. As a critical note, these calculations do not account for conductive heat losses via the wire-leads to that feed the heating system with current.
3.4. ENERGY-BALANCE MODEL

Figure 3.7: The power requirements for the full system, including fluid heating, conductive losses and radiative losses.

**ELECTRICAL EFFICIENCIES**

The expected efficiencies are calculated as the power required to heat the fluid, over the power required for the full system (fluid heating and losses), using equation 3.13, and shown in figure 3.8.

\[
\eta = \frac{P_{fl}}{P_{fl} + P_{cond} + P_{rad}}
\]  

(3.13)

Figure 3.8: The electrical power efficiency of the system, as a function of wall temperature and inlet pressure.

In figure 3.8 it is apparent that the maximum efficiency is attained at the highest pressure tested, combined with the lowest wall temperature. By contrast the highest wall temperature with the lowest pressure produces the least efficient mode of operation. As wall temperatures increase, the mass flow rates decrease, reducing the needed power flow to the fluid (see figure 3.4), whilst simultaneously increasing losses via conduction and convection (see figure 3.6).

Finally it is worth observing the very low efficiencies in the low-pressure cases, ranging from just under 50% to \( \approx 20\% \). Figure 3.4 shows a power request for the fluid of \( \approx 0.3\text{[W]} \), while the losses start at just over 0.3[W] and increase to nearly 1.2[W]. It remains however debatable if this efficiency value is of any importance: the
system has been designed to supply 7[W] of heating power, while the total system power is well below 1.5[W] for the maximum temperature and minimal pressure case. Therefore despite this very low efficiency, the system should have no trouble to function during those low-pressure situations.

3.4.3. **PROPELLANT EFFICIENCIES**

Next to power efficiency, the aerospace industry is probably even more interested in the propellant efficiency, or specific impulse \(I_{sp}[s]\). The specific impulse is calculated using equation 2.17, evaluating the force generated per unit of mass of propellant used. As using less mass to generate the same force increases the manoeuvring capacity of a space-vehicle, having a high \(I_{sp}\) value is often of higher importance than the power-efficiency. Figure 3.9 displays the computed \(I_{sp}\) values.

![Figure 3.9: The propellant efficiency, or \(I_{sp}\), of the system, as a function of wall temperature and inlet pressure.](image)

Note that changing the pressure does not influence the \(I_{sp}\). The \(I_{sp}\) values of all cases are superimposed (in figure 3.9 only the 0.5[bar] and 5.5[bar] are plotted).

The \(I_{sp}\) has been calculated using equation 2.17, whilst using equation 2.37 to calculate the assumed force. This equation already takes into account the increased boundary layer effects of the planar nozzle, so the values plotted in figure 3.9 are expected to be realistic.

However experimentally determined \(I_{sp}\) values such as those gathered by [15] show values reaching just over 100[s], with a nozzle height of \(100 \times 10^{-3}[\text{mm}]\), while the currently investigated system has a somewhat smaller height of \(75 \times 10^{-3}[\text{mm}]\). The expansion ratio for the current design is however much larger: it shows a value of 16.6, versus 9 used by [15].

According to the work of [23], the continuum approach for the diverging nozzle section can become problematic due to the very low pressures involved. Indeed, pressures of only \(\approx 235[\text{Pa}]\) remain after expansion in the 0.5[bar] feed pressure cases. The Knudsen number calculated for such pressures using equations 3.14 and 3.15 is well in excess of 10, therefore the continuum approach is not suitable. The \(I_{sp}\) values will therefore have to be experimentally checked, to assess if the calculated values are indeed correct.

\[
\lambda = \frac{\mu}{\rho} \sqrt{\frac{\pi M / N_A}{2 k_B T}} \tag{3.14}
\]

\[
Kn = \frac{\lambda}{H_{\text{nozzle}}} \tag{3.15}
\]

In these equations 3.14 and 3.15 \(M\) indicates the molar mass of water \(18[\text{kgmol}^{-1}]\), \(N_A\) indicate Avogadro's number \(6.022 140 857 \times 10^{23}[\text{mol}^{-1}]\) and \(k_B\) is the Boltzmann constant \((1.380 650 4 \times 10^{-23} [\text{JK}^{-1}])\).
The calculated force values shown in figure 3.10 will therefore also be uncertain for the lower pressure cases, due to the high Knudsen numbers at the end of the expansion in the nozzle.

![Figure 3.10: The produced force of the system](image)

In figure 3.10 the constant force per chamber temperature stands out. Previously, the velocity attainable by the fluid, as expressed in equation 2.30, should increase with the square root of the chamber temperature. However, this effect is nullified by the reduction in mass flow, visible in equation 2.34. As the force furthermore depends only on the pressure in the chamber and the expansion ratio, no effect of the temperature on the generated force is expected.

### 3.4.4. Energy-Balance Model in Review

The balance model discussed above provides a rather complete overview of the major design parameters of interest. Expected mass flows, power requirements, losses and efficiencies are all computed. Compared to the modelling efforts by [8], information on expected efficiencies and \( I_{sp} \) values are provided. The expected efficiency value of 50% that was assumed by [8] seems to underestimate the efficiency of the system.

Furthermore, [8] reported no specific impulse values, though he did report the expected thrust values. The values calculated using the computation method explained in section 2.2 show slightly lower thrust values, with the maximum thrust levels of 1.32[mN], as opposed to the thrust level of 1.4[mN] quoted by [8].

Key issues with VLM’s have yet to be investigated include the distribution of power throughout the heater, transients experienced when liquid starts to enter the system, and flow instabilities as experienced for instance by [16, 31]. Therefore fluid-flow effects such as spitting cannot be assessed yet.

This indicates the need for more complex models, able to investigate these phenomena. The first step to such a goal would be to introduce a 1D model, capable to calculate the temperature of the liquid, and able to judge key factors to ensure that only fully evaporated water may enter the nozzle.

### 3.5. Steady-State 1D Flow Model

As concluded in the previous section, the 1D model intends to divine the key factors to ensure full evaporation and therefore insuring the most efficient usage of the propellant. It will at first do so using a steady-state model.

Using the steady-state model, minimal wall temperatures, given the length of the heater, to attain complete evaporation can be assessed, for the intended pressure operation range. Similarly the average pressure drop over the heater is assessed, and its effect on the mass flow through the nozzle calculated. These calculations are combined with the IRT calculations to present a more accurate performance prediction of the VLM system.
An accurate (averaged) thruster behaviour model will allow designers to adjust heater length, based on better estimates of the flow velocities and residence times, account for an accurate measure of pressure drop over the heater, and the expected effects of various sizes and shapes of flow-interrupting pillars.

Next to these key factors to judge the performance of the VLM system, information on the flow such as Reynolds numbers, fluid velocities, vapour fractions and residence times are similarly calculated. They are presented in appendix C.

3.5.1. Approach

To facilitate straightforward modelling, the thruster system will first be investigated using the simplifications posed in section 3.1: the heating power is assumed to be applied via the silicon, heating the silicon to a uniform temperature.

Initially the investigation will focus on a simplified design, discounting the effect of the pillars on both heat flux coefficient as well as pressure drop. Initial (uncorrelated results) will briefly be discussed.

The layout and mass fluxes of the simplified model are closely related to the systems experimented upon by [16, 31], whose work is covered in greater detail in appendix B. Using the results of their reported experiments, a correlation factor for the heat flux coefficient in the two-phase regime can be calculated, which is the main unknown for the time-averaged heating process.

Next, temperature gradients in the silicon are calculated, to judge the need for a different heater power distribution, and put the near-constant wall temperature assumption to the test.

Finally, the effect of the designed diamond-shaped pillars (rhombi) is assessed, using the correlated model of the simplified structure as the baseline. This investigation will evaluate if lower wall temperatures or shorter heaters are allowed to attain complete evaporation when using rhombi, and whether this comes at a cost to other aspects of the thrusters performance.

3.5.2. 1D Time-Averaged Algorithm

Similar to the energy-balance model, the initial estimate of mass flow is performed using an assumed fully evaporated flow, at wall temperature and inlet pressure, using equation 2.34. Next, the length of the heater is divided in several short sections of length $\Delta x[m]$. Using the local pressure $p$ and local specific enthalpy $e$ of the fluid, fluid properties are determined using the steam tables recorded in XSteam [46]. The investigated properties are:

1. Temperature of the fluid
2. Saturation temperature as a function of pressure
3. Fluid vapour quality, the mass section of vapour (see equation 2.39)
4. Vapour volume fraction, the section of the volume occupied by vapour (see equation 2.40)
5. The averaged density of the fluid, for the mixed region based based on the vapour volume fraction and saturation properties of liquid and vapour.
6. The conductivity of the fluid, for the mixed region based based on the vapour volume fraction and saturation properties of liquid and vapour.
7. The viscosity, for the mixed region based on the volume fraction and saturation properties

The assessment of the properties mentioned above is a relatively straight-forward use of the material property tables. Please refer to appendix D for information on how the digitised steam tables are used.

As mentioned in section 2.4, averaging the fluid properties in micro-boiling-systems generally does not yield very accurate models, as opposed to tracking the position of the border between gas and the liquid phase, and using either gas or liquid properties. However the averaging of properties is believed to be a valid approach in this case, as this model attempts to only predict average power distributions and pressure drops, and does not lay claim to any predictions of flow oscillatory effects, spitting, or other transient effects.

Next, the 1D velocity $u$ of the fluid in the section in question is determined, using the mass flow rate based on equation 2.34, the density $\rho$, and the cross section $A_{cs}$ of the system.
Using this velocity, the residence time \( \dot{\theta} \) is determined. This indicates the time that passes as the fluid flows through the section of length \( \Delta x \) currently investigated.

\[
\dot{\theta} = \frac{\Delta x}{u} \tag{3.17}
\]

The pressure drop over the element length \( dx \) is computed by rewriting equation 2.11 to equation 3.18. Note that this equation does not include information on the effect of the rhombi, or other flow-interrupting pil-lars. The local viscosity \( \mu \) is determined using the steam tables, and the previously known local pressure and enthalpy values. The height \( H \) is based on the known dimensions of the system.

\[
\frac{\partial p}{\partial x} = -u \frac{12\mu}{H^2} \tag{3.18}
\]

The heat flux coefficient to the fluid is computed using equation 2.14, reprinted below for convenience, with \( \kappa \) the conductivity of the fluid based on the steam tables:

\[
h_{\text{conv}} = Nu \frac{\kappa}{D_h} \tag{3.18}
\]

The Nusselt number used in these equations is fixed at 6.0 based on the tables printed by [18]. The hydraulic diameter \( D_h \) is determined using equation 2.8, using the dimensions printed in appendix A.

Using the temperature difference between the fixed wall temperature \( T_w \) and the fluid temperature \( T \), the heat flux per unit of area is provided by equation 2.13. Using the area available for conduction as the internal perimeter \( \mathcal{P} \) of the heater multiplied with section length \( \Delta x \), this is converted to a heating power in equation 3.19.

\[
Q = h_{\text{conv}} (T_w - T) \mathcal{P} \Delta x \tag{3.19}
\]

Now using the residence time for the local section, as calculated with equation 3.17, the total energy influx is computed:

\[
\Delta E = Q \dot{\theta} \tag{3.20}
\]

Using the energy influx \( \Delta E \), and dividing that by the mass present in the volume, the specific enthalpy increase \( \Delta e \) is computed:

\[
\Delta e = \frac{\Delta E}{A_c \Delta x \rho} \tag{3.21}
\]

Adding this enthalpy increase to the already present enthalpy in the fluid, the fluid state and properties are recomputed for the section following the current section. Note that in this analysis the length-wise transfer of heat through the fluid itself is neglected.

### 3.5.3. Preliminary results

The algorithm as explained in section 3.5.2 and showed in Matlab-script in appendix H. Initial uncorrelated results are shown below.

<table>
<thead>
<tr>
<th>Wall temp [K]</th>
<th>( p_{in} = 0.5 ), BM</th>
<th>( p_{in} = 0.5 ), 1D</th>
<th>( p_{in} = 5.5 ), BM</th>
<th>( p_{in} = 5.5 ), 1D</th>
</tr>
</thead>
<tbody>
<tr>
<td>430</td>
<td>0.118</td>
<td>0.118</td>
<td>1.301</td>
<td>[-]</td>
</tr>
<tr>
<td>480</td>
<td>0.112</td>
<td>0.112</td>
<td>1.232</td>
<td>[-]</td>
</tr>
<tr>
<td>530</td>
<td>0.107</td>
<td>0.106</td>
<td>1.172</td>
<td>1.172</td>
</tr>
<tr>
<td>580</td>
<td>0.102</td>
<td>0.102</td>
<td>1.121</td>
<td>1.120</td>
</tr>
<tr>
<td>630</td>
<td>0.098</td>
<td>0.097</td>
<td>1.075</td>
<td>1.075</td>
</tr>
<tr>
<td>680</td>
<td>0.094</td>
<td>0.094</td>
<td>1.035</td>
<td>1.035</td>
</tr>
</tbody>
</table>
Table 3.2: Mass flow rates \(\text{[mgs}^{-1}\text{]}\), as calculated by the Balance model (BM) and the uncorrelated 1D model, where pressure drops are a (limited) factor. All pressures in [bar]

The mass flow rates determined lie very close to those determined using the Balance model, as is seen in table 3.2, due to the very limited pressure drop over the heater. At times the 1D model does report a slightly lower mass flow rate. For instance, the 630[K], 0.5[bar] case, or the 580[K], 5.5[bar] case. In these cases the mass flow rate was affected to some degree by the pressure drop, accounted for in the 1D model (see equation 3.18), while the balance model assumes a negligible pressure drop over the heater, and therefore a slightly higher mass flow rate.

Secondly the lack of a mass flow result for the 430[K], 5.5[bar] and 480[K], 5.5[bar] cases should be noted. These cases are predicted to not attain full evaporation. As such, the equation 2.34 is unable to provide correct results, and they are omitted from the table.

Studying the Reynolds numbers, the type of flow in the system can be determined. In section 2.1.1 estimates were provided using an inlet pressure of 1[bar] and mass flow rate of \(1 \times 10^{-6}\text{[kg}\text{s}^{-1}\text{]}\), resulting in Reynolds numbers varying from 0.63 to 32. The initial calculation yielded remarkably higher Reynolds numbers, especially so in the inlet channel. As the inlet channel is cut out of the same silicon block, it stands to reason that the fluid will be heated in this section as well. Consequently the fluid flows are seen to undergo partial evaporation in the inlet section, causing decreasing viscosities and consequently higher Reynolds numbers. The highest calculated Reynolds number is \(\approx 230\), still comfortably laminar.

As referenced to before, the temperature plots of figures 3.11a and 3.11b show the effect of increasing the feed pressure: in the 0.5[bar] case, the ‘boiling plateau’ of the two-phase regime lies at \(\approx 354.5\text{[K]}\), while that of the 5.5[bar] case lies at \(\approx 428.6\text{[K]}\).

The result of both the higher saturation temperatures and the higher mass flow rates of the 5.5[bar] case result
in a lack of complete evaporation for wall temperatures of 430[K] and 480[K]. Consequently, the fluid never grows beyond the saturation temperature.

The attaining of the wall temperature is clearly a process that requires a shorter length of the heater in the low-pressure case, in part due to the reduced mass flow. Secondly, the density in the 5.5[bar] case is 11.3 times larger at 2.60[kg m\(^{-3}\)] than the 0.5[bar] case at 0.23[kg m\(^{-3}\)] (evaluated at 473[K]). As the specific isobaric heat capacity \(c_p[J kg^{-1} K^{-1}]\) changes relatively little (increasing by \(\approx 10\%\) from 0.5 to 5.5[bar]), the amount of energy required to heat a volume element of the gas is significantly larger in the higher pressure case.

Figures 3.11c and 3.11d show the progress of evaporation. In both cases, the initial process is slower, indicated by a smaller inclination of the vapour mass fraction line. This is due to the faster fluid velocity in the inlet section, resulting in lower residence times, and less time for the heat to be transferred to the fluid. Of further note is the vapour mass fraction of the 480[K], 5.5[bar] case: about 90% of the latent heat was added to the fluid when it reached the end of the heater. Conversely, higher wall temperatures allow for a reduction of length of the heater, based on the average point of evaporation.

### 3.5.4. Correlations with experimental data

As suggested in section 2.4, creating generally-applicable two-phase flow and heat transfer models is not a trivial task. Based on the fact suggested by [18] that micro-flow single-phase heating is sufficiently modelled using macroscopic models, up to nano-meter systems, the main issue lies with the fidelity of the two-phase region models. Using the available knowledge presented on both the wall temperature of the heaters by [16, 31], as well as the visual data on the estimated average evaporation point, a heat-flux correlation coefficient can be created.

The goal of this correlation coefficient is to enhance fidelity of the expression for the heat transfer in the two-phase regime, allowing for a better prediction of the general performance by the steady-state 1D model. The affected equation for heat transfer is 2.13, where the correlation coefficient for the two-phase regime is added \((C_{tp}):\)

\[
h_{conv} = C_{tp} N u \frac{\kappa}{D_h} \quad (3.22)
\]

To adjust \(C_{tp}\) the 1D modelling algorithm is adjusted to the dimensions of the inlet section for [31], while it is adjusted to the full heater length of [16]. Simulations mimicking the reported experimental parameters concerning mass flow, wall temperature, and (if reported) pressures were conducted. If the pressures are not reported, a pressure estimate is selected. The coefficient \(C_{tp}\) is varied, until the resultant simulation mimics the visual data reported of the expected point of full evaporation.

Of note is the lack of correlation on the pressure drop: the choked-flow nozzle and very small dimension of the VLM heaters under study make the placement of a pressure sensor after the evaporation region very hard. As such, no knowledge of the pressure drops is available in literature, on fully evaporative micro-flows in low-mass-flux conditions.

**Cen Correlation**

The simplified design without heating rhombi as used so far is similar to the inlet section reported by [31].

As per the description explained in appendix B, [31] observe complete evaporation often before the end of then inlet section, though at times small droplets go beyond this section. This is paraphrased as an average evaporation point just before the end of the inlet section. Test parameters and dimensions used are described in table 3.3.
Table 3.3: Dimension and settings used for the correlation test.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate</td>
<td>2.33[mgs⁻¹]</td>
</tr>
<tr>
<td>Wall temperature</td>
<td>553[K]</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>293[K]</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>2.2[bar]</td>
</tr>
<tr>
<td>Heated length</td>
<td>4[mm]</td>
</tr>
<tr>
<td>Heated width</td>
<td>2[mm]</td>
</tr>
<tr>
<td>Heated height</td>
<td>0.12[mm]</td>
</tr>
</tbody>
</table>

In figure 3.12 the results for two average evaporation lengths are shown: the uncorrelated and correlated lengths. Note the very large difference: the (default) factor of 1.0 shows that on average the system would not be able to add half of the required latent heat to evaporate the fluid. The correlation factor of 2.75 shows an average evaporation point at approximately 90% of the heater length, therefore in agreement with the visual observations reported by [31].

**Chen correlation**

Similar to the prior correlation, correlating to the paper published by [16] has the benefit of the availability of visual images recorded of the operation of the VLM.

The pressures are not reported by [16]. As such, the pressures are estimated with the application of equation 2.34, based on the wall temperatures, the mass flow rate and the reported dimensions of the nozzle throat. This results in the test scenario with inlet temperatures held at 293[K], and the total heater length of 15[mm], though similar to the design by [8] a narrow inlet section precedes the wide heater section. All sections are set to the same wall temperature. Parameters are shown in table 3.4:

<table>
<thead>
<tr>
<th>Fully evaporated?</th>
<th>No</th>
<th>Yes</th>
<th>No</th>
<th>Yes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate</td>
<td>2.1[mgs⁻¹]</td>
<td>2.1[mgs⁻¹]</td>
<td>4.2[mgs⁻¹]</td>
<td>4.2[mgs⁻¹]</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>1.0[bar]</td>
<td>1.1[bar]</td>
<td>2.1[bar]</td>
<td>2.2[bar]</td>
</tr>
</tbody>
</table>

Table 3.4: Dimension and settings used for the correlation test.

As the design of this VLM is more complicated than the inlet section used from [31], please refer to appendix B for a fully detailed design drawing.

In figure 3.13 the comparison is shown between the studied cases without and with adjusted $C_p$ values. Next to the slope change observable in all cases due to the inlet-section ending up in the wide heater section, a
3.5. STEADY-STATE 1D FLOW MODEL

(a) Uncorrelated vapour mass fraction: \( C_{tp} = 1 \)

(b) Correlated vapour mass fraction: \( C_{tp} = 2.75 \).

Figure 3.13: The comparison of the length needed to attain an on-average evaporated flow, with the default correlation number on the left (a) and the correlated results on the right (b).

Clear difference between 3.13a and 3.13b is observable: in the former all cases fail to heat the fluid up to evaporation, in contrast to the reported visual observations. In the latter figure the cases reported as evaporated (see table 3.4) are similarly simulated as evaporated, while the cases where incomplete evaporation is reported, are indeed also not completely evaporated.

3.5.5. RESULTS OF CORRELATED TIME-AVERAGED 1D MODEL

Based on the results shown in figure 3.12 and 3.13, a factor of \( C_{tp} = 2.75 \) is used to adjust the heat flux into the two-phase region, and the simulations are re-investigated.

The operation ranges on wall temperatures and pressures shown previously in table 3.1 are investigated. To ensure a representative set of input parameters, the full temperature range is investigated with steps of 50[K]. Similarly a pressure for start-of-operations is used (5.5[bar]), a pressure for end-of-life operation (0.5[bar]), and two pressures representing performance expected during mid-life operation (2.0 and 3.0[bar]). Analysis of flow patterns (Reynolds numbers), mass flow rates, temperature distribution in the fluid, velocities and residence times, as well as generated thrust is performed.

Concerning flow patterns: all investigated cases showed laminar flow based on Reynolds numbers (< 260). The full investigation report is shown in appendix C. Here mass flow calculation results, temperature profiles, thrust estimates and specific impulse values will be discussed.

MASS FLOW RATES

Though the increased heat-flux does speed up the fluid velocities sooner, and consequently the pressure drops are slightly larger, the calculated mass flow rates are barely changed compared to the balance model, or the uncorrelated 1D model. The complete overview is provided in table 3.5.

The faster evaporation rate does however allow for the system to fully evaporate the flow for the 480[K], 5.5[bar] case, which was impossible for the uncorrelated model. Mass flow rates for this test are the same as those reported by the Balance model.

<table>
<thead>
<tr>
<th>Wall temp [K]</th>
<th>( p_{in} = 0.5 )</th>
<th>( p_{in} = 1.5 )</th>
<th>( p_{in} = 2.5 )</th>
<th>( p_{in} = 3.5 )</th>
<th>( p_{in} = 4.5 )</th>
<th>( p_{in} = 5.5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>430</td>
<td>0.118</td>
<td>0.355</td>
<td>0.591</td>
<td>0.830</td>
<td>[-]</td>
<td>[-]</td>
</tr>
<tr>
<td>480</td>
<td>0.112</td>
<td>0.336</td>
<td>0.560</td>
<td>0.784</td>
<td>1.008</td>
<td>1.232</td>
</tr>
<tr>
<td>530</td>
<td>0.106</td>
<td>0.320</td>
<td>0.533</td>
<td>0.746</td>
<td>0.959</td>
<td>1.172</td>
</tr>
<tr>
<td>580</td>
<td>0.102</td>
<td>0.305</td>
<td>0.509</td>
<td>0.713</td>
<td>0.917</td>
<td>1.120</td>
</tr>
<tr>
<td>630</td>
<td>0.097</td>
<td>0.293</td>
<td>0.488</td>
<td>0.684</td>
<td>0.879</td>
<td>1.075</td>
</tr>
<tr>
<td>680</td>
<td>0.094</td>
<td>0.282</td>
<td>0.470</td>
<td>0.658</td>
<td>0.846</td>
<td>1.035</td>
</tr>
</tbody>
</table>

Table 3.5: Mass flow rates [mg s\(^{-1}\)], as calculated with the correlated 1D model. All pressures in [bar]
Based on these mass flow numbers, and their similarities with those calculated when neglecting pressure drops, it comes as no surprise that the calculated pressure drops as a ratio of the inlet pressure are very small. Table 3.6 provides an overview for tested range of both relative and absolute pressure drops.

<table>
<thead>
<tr>
<th>Inlet pressure</th>
<th>Relative pressure drop</th>
<th>Absolute pressure drop</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>&lt;4.6 × 10^{-3}</td>
<td>2.3 × 10^{-3}</td>
</tr>
<tr>
<td>2.0</td>
<td>&lt;8.5 × 10^{-4}</td>
<td>1.7 × 10^{-3}</td>
</tr>
<tr>
<td>3.0</td>
<td>&lt;5.5 × 10^{-4}</td>
<td>1.6 × 10^{-3}</td>
</tr>
<tr>
<td>5.5</td>
<td>&lt;2.8 × 10^{-4}</td>
<td>1.5 × 10^{-3}</td>
</tr>
</tbody>
</table>

Table 3.6: Maximum pressure drops for the correlated models, tested at \(T_w = 680[K]\). Absolute pressures in [bar]

### Temperature Profiles

The increased correlation coefficient for the two-phase regime was already indicated to allow a larger range of evaporation, now also allowing the 480[K], 5.5[bar] to obtain full evaporation. Figure 3.14 shows the evolution of the average temperature through the heater.

The increasing inlet pressure shown in the sequence of plots shows the increase in saturation temperature. Seeing that the lowest wall temperature case of 430[K] with an inlet pressure of 5.5[bar] does not evaporate is therefore not surprising at all, as the remaining superheat is just \(\approx 1.5[K]\). A superheat of just over 50[K] is now indicated to be sufficient to fully evaporate the fluid and reach the wall temperature in the 5.5[bar] case (figure 3.14d).

![Temperature Profiles](image)

Figure 3.14: Fluid temperatures for various inlet pressures and wall temperatures
As one of the questions posed in the introduction was to determine what the minimum length of the heater needed to be, to ensure full evaporation, figure 3.14 seems to answer that question: for all investigated operating conditions, having a wall temperature of 480[K] (or ≈200[°C]) should be sufficient to ensure on average evaporation before half the length of the current heater. This boils down to a length of just 5[mm], including an inlet section of 1[mm].

However, this model details the length needed for the average point of full evaporation. In the real, time-dependent system, some liquid might surpass this point. Therefore spitting might more readily occur if the length of the heater is appreciably shortened.

**Forces and Specific Impulse Values**

Due to the relatively small pressure drops reported by the simulations, the mass flows have changed very little, if at all. Furthermore, as seen in figure 3.14 the temperatures of the vapours (for the cases where full evaporation occurred) reached the wall temperatures, so the assumption in the balance model of a chamber outflow at the wall temperature remains valid.

As equation 2.37 depends on both mass flow (which remains unchanged) and final velocity (which due to the final temperature reaching the wall temperature, and equation 2.30 remains unchanged), the reported thrust values in figure are nearly indistinguishable to those reported prior with the balance model in figure 3.10.

### 3.5.6. Silicon Temperature Gradient

Calculating the silicon temperature gradient is important as so far it has been assumed that the silicon has a uniform temperature. A shift in temperature is the result of a mismatch between the power flowing from the silicon into the fluid, and the power locally generated and fed into the silicon, by the electrical heaters. As stated in the start of section 3.5, the 1D model assumes that the heating power is uniformly distributed directly onto the silicon.

As the latent heat entails the largest part of the energy ‘consumption’ by the heating process, it is understandable that given the temperature plots shown in figure 3.14, most of the heating occurs well before half the heater has passed.

To evaluate the effect that this un-evenly distributed power has on the silicon, a model of the silicon base structure is set up, as seen in figure 3.15. The silicon wall temperature gradient is determined by assuming a uniformly distributed power influx. To do so, the system is assumed to attain the steady-state operating as described in the 1D steady-state model. Losses via conduction to the satellite structure, or via radiation to space, are not included in this evaluation. The silicon is modelled as a 1D steady-state system, where over every section of the heated wall, equation 3.24 is evaluated, graphically represented by figure 3.15.

![Figure 3.15: The power distribution computed for each section length Δx](image)

The blue square marked silicon represents a volume element, spanning the full width of the silicon heater, and of a height comprised of the combined bottom and top thickness of the structure. The cross-section formed with these dimensions is dubbed $A_{si}[m^2]$. The heater is subsequently sectioned in small lengths $\Delta x$, corresponding to the $\Delta x$ lengths used for the fluid model. This entails that for every section, a known power is being drawn into the fluid, power flow $Q_1[W]$, as calculated in the 1D fluid model. Conversely, by finishing the 1D fluidics model, the total power draw by the fluid is known, as the summation of the powers drawn by
the individual sections. The power input per heater section $Q_2 [\text{W}]$ is then computed as the average of the total supplied power:

$$Q_2 = \frac{\sum_1^n (Q_1)}{n}$$

(3.23)

Here $n$ represents the number of elements used. Heat flow $Q_3 [\text{W}]$ represents the heat flowing from the element in question, to the element closer to the start of the heater, while $Q_4 [\text{W}]$ represents the heat flowing in from the next element, which will be closer to the nozzle. As the system is considered to be time-independent, the summation of energy flows must be zero:

$$0 = -Q_1 + Q_2 - Q_3 + Q_4$$

(3.24)

Using equation 3.25, the required temperature difference to the prior element can be assessed, while equation 3.26 determines the temperature difference with the next element. In these equations, $\kappa_{\text{Si}} [\text{Wm}^{-1}\text{K}^{-1}]$ indicates the silicon conductivity.

$$\Delta T_{\text{left}} = \frac{Q_3 \Delta x}{\kappa_{\text{Si}} A_{\text{Si}}},$$

(3.25)

$$\Delta T_{\text{right}} = \frac{Q_4 \Delta x}{\kappa_{\text{Si}} A_{\text{Si}}},$$

(3.26)

If we pose that the first element has no further elements to its left, the temperature step shown in equation 3.25 must be zero. This allows equation 3.24 and 3.26 to be rewritten to:

$$\Delta T_{\text{right}} = \frac{(Q_1 - Q_2) \Delta x}{\kappa_{\text{Si}} A_{\text{Si}}},$$

(3.27)

As for the succeeding element, the former right-sided temperature difference is now the known left-sided temperature difference, and the equation can be iterated on until the final element is reached:

$$\Delta T_{\text{right}} = \frac{(Q_1 - Q_2 + \frac{\Delta T_{\text{left}} \kappa_{\text{Si}} A_{\text{Si}}}{\Delta x}) \Delta x}{\kappa_{\text{Si}} A_{\text{Si}}},$$

(3.28)

The resultant temperature gradients are provided in figure 3.16. Note that only the highest wall-temperature cases are printed, across all tested pressures, as these were determined to have the largest absolute temperature shift.

As the temperature shifts visible in figure 3.16 are in the order of 3.1[K] or less, the assumption of the uniform silicon temperature will hold. As the mass flow increases proportionally to the inlet pressure, the higher heat flux to the fluid at higher pressures causes an understandable larger temperature differential in the silicon.

Based on the limited temperature gradients no complicated power-input distribution methods will have to be included in the heating system, relaxing the design criteria. Similarly, easier (external) heat influx methods may be considered if internal heating proves to be too difficult to realise.

### 3.5.7. Effects of Rhombi on Fluid Flow

The analysis of the system so far is aimed at a simplified design. However, the design proposed by [8] utilises heat-transfer enhancing pillars. These pillars, denoted as ‘rhombi’ because of their diamond-shaped horizontal cross-section, have an effect on both the pressure drop along the heater, as well as the heat transfer coefficient.
3.5. Steady-state 1D Flow Model

Figure 3.16: The temperature profile in the silicon, for the maximum shift of $T_w = 680\text{[K]}$

**Pressure drop with Rhombi**

The pressure drop including the rhombi was calculated by [8] using the Ergun equation 3.29, as mentioned in chapter 1. However, the origin of this packed-bed computation seems to be a possibly turbulent flow field, as suggested by [50].

\[
\Delta p = 150 \mu \frac{L}{D_p} \left(1 - \epsilon\right)^2 \frac{u_s}{\epsilon^3} + \frac{1.75 L \rho}{D_p} \left(1 - \epsilon\right) \frac{u_s |u_s|}{\epsilon^3}
\]  
(3.29)

In the Ergun equation, $D_p$ represents the characteristic diameter of the packed-bed elements, in this case the rhombi, while $\epsilon$ represents the porosity of the system, or the fraction of the volume of the heater not occupied by the packed bed elements. Next $u_s$ represents the ‘superficial’ velocity, or the average velocity the fluid would attain if no packed bed elements were present in the fluid, which is calculated as in equation 3.30:

\[
u_s = \frac{\dot{m}}{\rho A_{cs}}
\]  
(3.30)

Conversely, the average speed while accounting for the present rhombi is calculated as:

\[
u = \frac{\dot{m}}{\rho A_{cs} \epsilon}
\]  
(3.31)

The parameters tested by [8] are listed in table 3.7.

<table>
<thead>
<tr>
<th>Property</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow rate $\dot{m}$</td>
<td>1 [mgs$^{-1}$]</td>
</tr>
<tr>
<td>Porosity $\epsilon$</td>
<td>0.67</td>
</tr>
<tr>
<td>Particle diameter $D_p$</td>
<td>$40 \times 10^{-3}$[mm]</td>
</tr>
<tr>
<td>Water viscosity $\mu$</td>
<td>$2.82 \times 10^{-3}$[Pas]</td>
</tr>
<tr>
<td>Density of fluid $\rho$</td>
<td>958.4[kgm$^{-3}$]</td>
</tr>
<tr>
<td>Length $L$</td>
<td>8.95[mm]</td>
</tr>
<tr>
<td>Cross section area $A_{cs}$</td>
<td>$4.5 \times 10^{-7}$[m$^2$]</td>
</tr>
</tbody>
</table>

Table 3.7: Test parameters used by [8] with the Ergun equation

The result of the application of these parameters to equation 3.29 is 201.1[Pa], a far cry from the 1.28[bar], or $1.28 \times 10^5$[Pa] presented by [8].
According to [51], a better fit to the system is the Kozeny-Carman equation, seen in equation 3.32.

\[ \Delta p = \frac{180\mu}{\Phi_s^2 D_p^2} \frac{(1 - \epsilon)^2}{\epsilon^3} u_L \]  

(3.32)

Equation 3.32 uses \( \Phi_s \) as a measure of the 'sphericity' of the particles, or to manner in which they resemble spheres. Previously [8] presumed the rhombi to act as round pillars, and as such this assumption will similarly be used, and the sphericity \( \Phi_s \) will be set to unity. Using the same parameters (see table 3.7), a pressure drop of 238.6 [Pa] is computed, similar to the result of the Ergun equation.

Note however that the pressure drop calculated using equation 3.18 and the same parameters amounts to only 3.1 [Pa]. Therefore it can be concluded that the pressure drop is duly influenced by the pillars.

The algorithm introduced in section 3.5.2 is therefore appended with equation 3.32 to allow for a computation accounting for pressure drop per section length \( \Delta x \). For these computations, the porosity of 0.67 is maintained, though the hydraulic-diameter equivalent of for the cross-sectional area of the pillars is used: \( D_{p,h} = 63.2 \times 10^{-3} \) [mm].

**Heat flux with Rhombi**

As mentioned in the start of section 3.1, the research by [40] suggests that the Nusselt number for flows where pillars are placed to increase mixing can double. As such, when the system is simulated while accounting for the presence of the Rhombi, next to the new pressure-drop calculations the Nusselt number is also doubled to 12, next to also taking into account the correlation factor previously determined, as seen in equation 3.33:

\[ h_{\text{conv}} = 2 C_{ip} \frac{Nu}{D_h} \]  

(3.33)

Note that the correlation factor is only active in the two-phase flow region, in single-phase regions it is 1.

**3.5.8. Simulation results of Rhombi-model**

The resultant simulation behaviour is analysed below, with respect to mass flow rates, pressure drops, temperature profiles, thrust values and specific impulses. For the full analysis, see appendix C.

**Mass flow rates**

The mass flow rates are very similar to the previously mentioned values. For the higher temperature cases, a small decrease in mass flow rate does become apparent, as seen when comparing table 3.8 to table 3.5.

<table>
<thead>
<tr>
<th>Wall temp [K]</th>
<th>( p_{in} = 0.5 )</th>
<th>( p_{in} = 1.5 )</th>
<th>( p_{in} = 2.5 )</th>
<th>( p_{in} = 3.5 )</th>
<th>( p_{in} = 4.5 )</th>
<th>( p_{in} = 5.5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>430</td>
<td>0.113</td>
<td>0.350</td>
<td>0.587</td>
<td>0.825</td>
<td>[-]</td>
<td>[-]</td>
</tr>
<tr>
<td>480</td>
<td>0.106</td>
<td>0.330</td>
<td>0.554</td>
<td>0.778</td>
<td>1.003</td>
<td>1.227</td>
</tr>
<tr>
<td>530</td>
<td>0.100</td>
<td>0.313</td>
<td>0.526</td>
<td>0.740</td>
<td>0.953</td>
<td>1.117</td>
</tr>
<tr>
<td>580</td>
<td>0.095</td>
<td>0.298</td>
<td>0.502</td>
<td>0.706</td>
<td>0.910</td>
<td>1.114</td>
</tr>
<tr>
<td>630</td>
<td>0.090</td>
<td>0.285</td>
<td>0.480</td>
<td>0.676</td>
<td>0.872</td>
<td>1.067</td>
</tr>
<tr>
<td>680</td>
<td>0.086</td>
<td>0.273</td>
<td>0.461</td>
<td>0.650</td>
<td>0.838</td>
<td>1.026</td>
</tr>
</tbody>
</table>

Table 3.8: Mass flow rates [kg/s], as calculated with the rhombi 1D model. All pressures in [bar]

The cause, the pressure drop over the heater, is shown in figure 3.17.

It should be noted that the pressure drops have increased significantly compared to the prior iterations, as best indicated by table 3.9.

<table>
<thead>
<tr>
<th>Inlet pressure</th>
<th>( (p_{in} - p_c)/p_{in} )</th>
<th>( p_{in} - p_c )</th>
<th>( (p_{in} - p_c)/p_{in} ) (R)</th>
<th>( (p_{in} - p_c)/p_{in} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5</td>
<td>&lt;4.6 × 10^{-3}</td>
<td>2.3 × 10^{-3}</td>
<td>9.3 × 10^{-2}</td>
<td>4.7 × 10^{-2}</td>
</tr>
<tr>
<td>2.0</td>
<td>&lt;8.5 × 10^{-4}</td>
<td>1.7 × 10^{-3}</td>
<td>2.4 × 10^{-2}</td>
<td>4.7 × 10^{-3}</td>
</tr>
<tr>
<td>3.0</td>
<td>&lt;5.5 × 10^{-4}</td>
<td>1.6 × 10^{-3}</td>
<td>1.6 × 10^{-2}</td>
<td>4.7 × 10^{-3}</td>
</tr>
<tr>
<td>5.5</td>
<td>&lt;2.8 × 10^{-4}</td>
<td>1.5 × 10^{-3}</td>
<td>8.4 × 10^{-3}</td>
<td>4.6 × 10^{-2}</td>
</tr>
</tbody>
</table>
3.5. **Steady-state 1D flow model**

![Diagram of normalised pressure drops](image)

(a) $p_{in} = 0.5 \text{[bar]}$

(b) $p_{in} = 2.0 \text{[bar]}$

(c) $p_{in} = 3.0 \text{[bar]}$

(d) $p_{in} = 5.5 \text{[bar]}$

**Figure 3.17**: Normalised pressure drops in the heater with rhombi, for various inlet pressures and wall temperatures

### Table 3.9: Maximum pressure drops over the heater for the no-rhombi versus rhombi (R) including model, tested at $T_w = 680 \text{[K]}$. All pressures in [bar]

Based on these results, adding the rhombi leads to a small loss of expected performance due to the reduction in final chamber pressure, reducing the available pressure prior to the nozzle when comparing to the feed-pressure. However, the largest relative loss occurs of pressure is less than 10%, occurring only for the end-of-life case of a storage pressure of 0.5[bar] see in figure 3.17a, and still considerably less than the expected 20% loss occurring throughout the operating range according to [8].

#### Temperature profiles

Though the heat-flux coefficient has doubled in the case with Rhombi compared to the case without rhombi, it’s effect on most temperature-profiles is minimal, as seen when comparing the case with rhombi shown in figure 3.18 and without rhombi, figure 3.14. As the effect of the rhombi does not become apparent until the inlet section (the first 10% of the heater length) has passed, the addition of this measure on the low-pressure cases is relatively small.

In the figure 3.18d a perceptible difference compared to figure 3.14d is noticeable though: the case of the rhombi-heater with a wall temperature of 480[K] shows an appreciably shorter required length to superheat, compared to the rhombi-less case.

The pillars produce a trade-off: the required length to evaporate the fluid is reduced, while the pressure drop over the heater is increased.

Of note here is that the transient effects such as bubble-explosions and flow oscillations will most likely be drastically influenced by the presence of rhombi, for instance due to the effect observed by [31] of bubble explosions occurring at sharp angles in the fluid. Furthermore, the rhombi will increase the chance that
small un-evaporated liquid droplets will hit a heated wall and subsequently still evaporate, as opposed to being carried along by the vapour flow through the nozzle, possibly influenced by the Saffman force [33].

FORCES AND SPECIFIC IMPULSE VALUES

As the mass flux is reduced due to the pressure drops, especially at higher temperature flows, the reported force values actually drop off slightly for increasing temperatures, as seen in figure 3.19. The effect however is minimal, when comparing figure 3.19a to 3.16. Similarly, the specific impulse is only slightly reduced from the balance model figures, as is apparent when comparing figure 3.19b to 3.9, as the former shows $I_{sp}$ values up to just below 130[s], while the latter just supersedes this value.

3.5.9. SILICON TEMPERATURE GRADIENT (RHOMBI CASE)

Finally the silicon temperature gradient investigation executed prior to the correlated model without rhombi, is repeated for the case with rhombi. As seen in figure 3.20, the gradient magnitude has increased. Due to the higher heat flux coefficient in the two-phase regime, the heat is transported into the fluid in a smaller length of heater. Consequently, the total power the heater conducts into the fluid (which is approximately unchanged, due to the very small mass flow rate changes) is now concentrated in a shorter section. As a result, a larger gradient in the silicon must be maintained in order to transport all the needed heat from the end of the heater to the sections where the heat is most needed.

Comparing figures 3.20 to 3.16 the difference is certainly noticeable (≈4[K] with Rhombi as opposed to ≈3.1[K] without Rhombi), but still limited enough to allow the use of the uniform-wall-temperature assumption.

Next to the investigated steady-state temperature gradients, the relatively large conductivity of the silicon allows for transient large heat fluxes that might occur during explosive bubble evaporation to have relatively
3.5. **Steady-state 1D flow model**

Using the balance model, an overview of the system behaviour for all operating conditions is quickly obtained. The 1D steady-state model described in this section adds to this the knowledge of the steady-state fluid behaviour, identifying minimal operating temperatures per input pressure, quantifying the pressure drop and consequent thrust reduction, both for heaters where the rhombi are fitted, as those without the rhombi.

Based on the models, a safe wall temperature value to ensure evaporation has been determined to be 480[K]. The expected pressure drop of the steady-state system are minimal, both for cases with and without rhombi, and as such the thrust values have not decreased appreciable from the values determined in section 3.4. The silicon temperature variation is determined to be very small, while the effect of rhombi on both pressure drop (small increase) and heat transfer (increase) have been determined.

Concerning the design, several lessons can be learned from this model alone:

1. Pressure reduction in the chamber is very limited, especially for cases without rhombi.
2. Using a wall temperature of $\approx 480[K]$ should provide sufficiently fast heating to the fluid

3. Limited residence times hint at fast responses, though this is to be confirmed using time-dependant modelling

As mentioned in point 3, start-up behaviour is the next knowledge hurdle to be cleared, to better predict the system behaviour during the design phase. Time-dependant behaviour of interest is comprised of (among others):

1. Start-up requirements
2. Spitting
3. Flow and pressure oscillations

To investigate the first of the remaining questions, modelling effort will continue with the 1D transient flow model.

3.6. **Transient 1D Flow Model**

As concluded in the previous section, the 1D steady-state model is able to convincingly calculate a multitude of parameters, but provides no knowledge on the start-up behaviour of the system. To this extent, a transient 1D model is created.

In a time-dependent experimental study of flow-boiling, such as performed by [16] or [31], visual analysis shows that at times a clear separate-phase system emerges. The study performed by [16] remarks the snake-flow profile, previously shown in figure 2.9, as one of the cases where liquid exited the system through its nozzle. With snake-flow, a clearly separate liquid path right through the middle of the heater is indicated. This type of flow is shown in an abstract manner in figure 3.21, where the blue filled region indicates snake flow, and the slanted green lines the uniform front approach.

An aspect of the steady-state 1D model is the assumption that the fluid has uniform properties over the full cross-section of the system. This approach is shown as the uniform-front approach. As the flow patterns average out over time, this is seen as an acceptable simplification.

In a time-dependent study, the interface-region between phases is an important parameter. To understand when spitting occurs, the interface must be tracked to see liquid entering the nozzle. As such, a model is called for where the progress of the liquid phase during start-up conditions is tracked, while the displacement of the surrounding vapour can be simplified.

A full 2D or 3D FEM calculation would in theory be an appropriate modelling technique. However, the large computational effort and uncertainties with respect to validity of different methods call for an investigation of analytical options.

To allow a calculation of the liquid-vapour interface, using an analytical model, 1D motion must be assumed. Two options persist for this 1D motion: a uniform front approach similar to the steady-state model, or a snake-flow approach.

If the uniform front approach is used, the liquid entering from the inlet channel into the heater will act as a piston, compressing what little vapour is created between the liquid front and the nozzle, quickly raising the pressure and ensuring that no liquid can enter the nozzle.

By contrast, if the snake-flow pattern is used, simplified to a straight flow with the cross-sectional dimensions of the inlet channel, a test to see if the evaporation speed is sufficient is created. If the evaporation speed is indeed sufficient, it will raise the chamber pressure via evaporation, to ensure that the chamber pressure will quickly reach the inlet pressure. As a consequence, the pressure driving the liquid forward will be countered.

The limit at which this occurs may be considered the minimal start-up silicon temperature.

3.6.1. **Transient 1D Model Algorithm**

To assess the dynamics of the system, the transient model assumes that the liquid that has entered the system acts as a single increasing or decreasing body of mass, of a width of the inflow-channel. This is shown in the
simplified overview drawing if figure 3.21. As such, when attempting to assess the rate of acceleration, mass changes have to be taken into account, leading to the full version of Newton’s second law: equation 3.34.

\[
\frac{\partial^2 (mx_L)}{\partial t^2} = \Sigma F \tag{3.34}
\]

The mass in the system is defined as in equation 3.35. The changing mass is reasoned to be accurate enough if feed-lines of the VLM are flexible, and the mass in those lines will therefore play a lesser role. Here \(x_L\) [m] represents the inflow distance into the heater, \(W_L\) [m] the width of the liquid flow, \(H\) [m] the height, and \(\rho_L\) [kgm\(^{-3}\)] the density of the liquid, assumed constant at \(\rho_L = 10^3\) [kgm\(^{-3}\)]. Finally, the thinner inlet section is neglected in this analysis, to simplify the algebra and acceleration derivations.

\[
m = \rho_L W_L H x_L \tag{3.35}
\]

Forces acting on the fluid consist of inlet pressure forces accelerating the fluid, while outlet pressure (chamber) forces with friction forces based on liquid motion decelerate the fluid.

\[
\Sigma F = W_L H (P_{in} - P_c - P_{\mu, L}) \tag{3.36}
\]

The vapour properties are determined based are assumed to be approximately uniform throughout the region occupied by vapour, while the temperature is assumed to lie at at the wall temperature. The density is determined using the Ideal Gas Law (IGL), using equation 2.23, repeated here for convenience:

\[
\rho_v = \frac{p}{R_s T}
\]

To compute the density of the vapour, a mass balance for the vapour mass is set up:

\[
\frac{dm_v}{dt} = \dot{m}_{\text{evap}} - \dot{m}_{\text{nozzle}} \tag{3.37}
\]

The evaporation mass flow is determined using a constant temperature differential between liquid and wall. As the major portion of the heat needed to evaporate the fluid is the latent heat, the saturation temperature is determined to find the temperature gradient:

\[
\Delta T_{\text{evap}} = T_w - T_{\text{sat}} \tag{3.38}
\]

The heat flux is determined by combining equation 2.14 with the available heat-transfer area (\(2W_L x_L\)):
\[ P_{\text{evap}} = \Delta T_{\text{evap}} \frac{NhKL}{D_h} 2W_Lx_L \quad (3.39) \]

Note that in equation 3.39 the liquid conductive properties are used. As liquid in contact with heated surfaces will superheat and provide vapour at the nearest liquid-vapour interface, or form a new vapour embryo, this approach is used to determine the transient heat flux model.

The total mass evaporation (all assumed to occur at the front of the liquid) is then determined by dividing the available power by the power required to evaporate 1 kg of liquid, from inflow temperature

\[ m_{\text{evap}} = \frac{P_{\text{evap}}}{c_{p,L}} \Delta T_L + e_{LH} \quad (3.40) \]

The outflow is calculated using equation 2.34, where the prior time-iteration calculated chamber pressure is used (or the initial value).

The newly calculated total vapour mass is assumed uniformly distributed in the chamber volume, to allow for a density calculation of equation 3.41.

\[ \rho_V = \frac{m_V}{WHL - W_LHx_L} \quad (3.41) \]

Recomputing the density to the pressure, relates the chamber pressure that is to be used in the next time iteration:

\[ p_c = \rho_V R_s T_c \quad (3.42) \]

Equation 3.42 is of course a rewritten version of equation 2.23.

The viscous forces due to liquid velocity are calculated based on the liquid inflow length \( x_L \), and constant properties:

\[ F_{\mu,L} = 12 \frac{H}{12} x_L \]

Assuming a uniform liquid flow cross-section, the algebraic derivation of the acceleration term based on liquid mass and position is simplified. The algebraically derived speed is shown in equation 3.44, while the acceleration is shown in equation 3.45.

\[ \frac{\partial (m_Lx_L)}{\partial t} = 2 \rho_L W_L H \left( \frac{\partial x_L}{\partial t} \right) x_L \quad (3.44) \]

\[ \frac{\partial^2 (m_Lx_L)}{\partial t^2} = 2 \rho_L W_L H \left( \frac{\partial^2 x_L}{\partial t^2} \right)^2 + \left( \frac{\partial x_L}{\partial t} \right)^2 \quad (3.45) \]

Accelerations are determined using the sum of forces as in equation 3.36 and the model for acceleration of the liquid as computed in equation 3.45. The resultant force balance is shown in equation 3.46:

\[ \frac{\partial^2 x_L}{\partial t^2} = \frac{5P}{2\rho_L H^2 \pi} \left( \frac{\partial x_L}{\partial t} \right)^2 \quad (3.46) \]

Using a time-stepping schematic, and initial states (position, velocity, pressure in the chamber), equation 3.46 is used to determine the velocity and subsequent position of the system.

Note that a correction will be added to this time-stepping scheme to account for fluid evaporated: the velocity of the liquid inflow front \( \frac{\partial x_L}{\partial t} \) is reduced by the mass evaporation speed \( m_{\text{evap}} \)

\[ \frac{\partial x_L}{\partial t} = \frac{\partial x_L}{\partial t} - m_{\text{evap}} \rho_L W_L H \quad (3.47) \]
This consequently only influences to penetration length of the liquid, not the speed of the liquid body.

3.6.2. RESULTS OF TRANSIENT 1D MODEL

Again the most difficult operating points are evaluated based on the balance model results (see section 3.4.4), using an inflow pressure of $p_{in} = 5.5 \text{ [bar]}.$ Several wall temperatures are tested, while the system uses a start-up chamber of $p_c = 1 \text{ [Pa]}$, or $p_c = 10^{-5} \text{ [bar]}.$ The results for the inflow length are shown in figure 3.22a, while the pressure progression is shown in figure 3.22b.

Figure 3.22 shows a comparison between the normalised liquid inflow distance, as a ratio of the full system length, and the normalised pressure (normalised to feed-pressure). The cases where the pressure runs short of that value correspond to the cases where liquid enters the nozzle before back-pressure can sufficiently build-up. This occurred for wall temperatures of 430 and 440[K], while 450[K] appeared to be a sufficient wall temperature to ensure enough evaporation, to increase the chamber pressure up to the inflow pressure.

The 470[K] case showed a similar response to the 450[K] case, but the pressure build-up in the chamber was markedly quicker, owing to the increased speed of evaporation. This also led to a smaller inflow length of the liquid column.

The 570[K] response should be noted as interesting, but not representative of expected behaviour. In this case, the very high wall temperature ensured that evaporation was fast enough to quickly force the liquid back, allowing the length of the column to oscillate (see figure 3.22a) as the chamber pressures briefly peaked above the inlet pressure (see figure 3.22b).

Though based on the work presented in chapters 2 and B oscillatory flow is expected, the current model is insufficient to perform these calculations: this model assumes the liquid to consist of a rigid column that can grow or shrink back into its origin. In reality, liquid water when presented with such a countering pressure, will deform.

Nonetheless the presented transient model can be used to judge if sufficient start-up conditions are met to ensure full evaporation.

![Figure 3.22](image)

(a) Normalised inflow length of the liquid column ($x_L$).

(b) Transient chamber pressure, normalised to inlet pressure.

Figure 3.22: Transient mode results for the 5.5[bar] inflow pressure

The steady-state 1D model is applied on the same conditions, to judge whether it would judge the same operating conditions as manageable. To do so, both the model with as well as the model without rhombi are tested. Results are shown in figure 3.23. With the system not including the rhombi (figure 3.23a), a slightly higher wall temperature of 455[K] is required, while the response of the system with rhombi (figure 3.23b) matches the predictions of the transient model.

3.6.3. REVIEW OF TRANSIENT 1D MODEL

Figure 3.22 shows that given a wall temperature of at least $T_w = 450[K]$ will ensure a stable operation point. This result is correlated to the steady-state model, where the same wall temperature is indeed shown to allow
full evaporation.

However, both models use a wide set of assumptions: the steady-state model uses mixing phases, and a uniform front approach, while the transient model uses a separate-phase, snake flow approach.

The main drawback of analytic models such as those shown here is therefore that assumptions on the flow pattern will have to be made. If the fluid does indeed behave as reasoned, the models should provide a very interesting correlation. However, if different flow patterns arise [such as the other patterns as observed by [16], or annular, slug or mist-flows (see section 2.4)], the model has very little predictive power.

In this case the transient model is expected to have reasonable correlative ability up to the point where the fluid flow starts to reverse. At that point, the assumption that the fluid can be modelled as a growing or shrinking 'bar' is no longer valid: the fluid front might recede, but that will simply cause the fluid to spread in the inlet section of the heater, increasing the area covered by liquid.

This gives rise to questions on where these liquid droplets go next. If they are propelled into the nozzle, this will lead to a reduced propellant efficiency.

The transient model has therefore not been able to predict the remaining two fluid-flow behaviours, that need to be known to further improve VLM designs:

1. Spitting
2. Flow and pressure oscillations

3.7. CONCLUSIONS ON ANALYTICAL MODELLING

This chapter has covered a wide array of subjects. Initially the currently designed heating method, using heating wires suspended in the middle of the flow, is judged based on simple thermal (section 3.1) and mechanical models (section 3.2). Next, a reverse-flow restrictor is proposed (section 3.3).

Two types of steady-state modelling are applied. First a balance model is applied (section 3.4), akin to the analysis performed by [11, 13, 15], though augmented with assessments of efficiency of both electrical heating systems as well as propellant usage. Secondly a 1D fluid flow model is applied (section 3.5), using correlations with two published papers ([16, 31]), to assess temperature distributions in both fluid and silicon. This model allows a test of minimal wall temperatures needed to ensure full evaporation of the fluid, as well as an assessment of the demands placed on the distribution of power influx into the system via the electrical heaters.

Finally an initial assessment of the dynamic behaviour during start-up conditions is provided by the time-dependent 1D flow model (section 3.6).
Table 3.10: Models detailed in this section, with knowledge attained.

<table>
<thead>
<tr>
<th>Model</th>
<th>Resultant knowledge</th>
<th>Section</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heater wire thermal analysis</td>
<td>Temperature distribution in heater wires</td>
<td>3.1</td>
</tr>
<tr>
<td>Heater wire mechanical analysis</td>
<td>Stresses applied on heater wires</td>
<td>3.2</td>
</tr>
<tr>
<td>Reverse flow investigation</td>
<td>Possibilities to reduce reverse flow</td>
<td>3.3</td>
</tr>
<tr>
<td>Energy balance model</td>
<td>Minimal power usage, efficiency, propellant efficiency</td>
<td>3.4</td>
</tr>
<tr>
<td>1D steady state model</td>
<td>Pressure drop, temperature distribution in fluid and silicon</td>
<td>3.5</td>
</tr>
<tr>
<td>1D transient model</td>
<td>Minimal wall temperature for start-up-conditions</td>
<td>3.6</td>
</tr>
</tbody>
</table>

Based on the work presented some observations are in order:

1. Move the heating wires from a suspended position, to the floor of the fluid channel, as currently little to no efficiency is gained, while a large amount of potentially debilitating failure points are added to the system (see section 3.1 and 3.2).

2. In literature, several reverse flow restrictions are mentioned, of which the Tesla valve seems one of the more flexible principles. Extra analysis of the single-phase flow inside this element would be recommended (see section 3.3).

3. Using the proposed mounting method, system efficiencies ensure that the power requirements reside well within the stated mission limits (see section 3.4).

4. Based on the steady-state 1D, a minimal wall temperature of 480[K] is selected, to ensure evaporation in all pressure-inlet scenario’s, ranging from 0.5 to 5.5[bar] (see section 3.5).

5. The diamond-shaped pillars, or rhombi, contribute to a larger pressure drop (up to 10% in end-of-life cases of inlet pressures of 0.5[bar]), while also shortening the heater length or temperature needed for evaporation (see section 3.5).

6. Similarly to conclusions reached with the steady-state model, the transient 1D model shows that a heater temperature of 480[K] is sufficient to ensure that a snake-flow-type of liquid inflow is prevented from reaching the nozzle structure, and causing spitting (see section 3.6).

Though the steady-state assumption used for most of the models presented here might be valid if averaged over sufficient time, the knowledge available in literature (see chapter 2) shows that severe flow oscillations may occur, that might drive liquid into the nozzle.

Similarly, in the case of the transient model, an assumed flow pattern is posed (snake-flow). Though this has shown to be a possible challenging scenario based on literature review, the current model uses a simplified evaporation system, where evaporation only occurs at the front of the simulated liquid column penetrating into the heater structure.

What if a nucleation starts in the middle of the flow, and liquid gets propelled forward? The current model has no way of predicting such an occurrence.

Therefore, in order to be able to assess heater performance and sensitivity to design changes, and more importantly, the odds of spitting and the effects of pressure and fluid flow oscillations given a design layout, a 2D time-dependent model is called for. This model is intended to answer the remaining questions.

1. How will pressure and flow velocity oscillations affect VLM functioning

2. Does the design require adjusting to prevent spitting, and if so, how?
First-principle based model studies

As concluded in chapter 3, the study of pressure and flow oscillations in the current VLM require a study that does not predetermine the fluid flow behaviour. Analytical steady-state and transient models therefore fall short as possible venues. The first-principle method allows for such an ‘open-minded’ modelling approach, as the fundamental principles of fluid-flow behaviour introduced in chapter 2 are ideally left to behave ‘as they wish’. However the study of evaporative two-phase micro-flow models has not fully matured, at least not to the point where models are readily available and able to be used on generic designs to judge system behaviour. Therefore, this chapter will perform tests of modelling options, ranging from an available existing modelling approach, to novel two-phase flow modelling approaches pioneered in this thesis.

To perform the tests of modelling methods, two modelling scenario's are introduced (see section 4.1). The first scenario is an abstract design domain, with (if possible normalised) design variables and fluid properties, to test the basic functioning of simulations. The second scenario will be a more life-like case, adhering to the dimensions of the current VLM design stated in appendix A, as well as using realistic liquid properties.

In section B.2 of appendix B the possibilities concerning first-principle finite-volume modelling of evaporative two-phase flows are expanded. Given the pre-existing knowledge of the COMSOL MultiPhysics program within the research department of 3mE at the Technical University of Delft, the COMSOL-proposed phase-field model has been selected as the first first-principle method to be tested. The applications of fluid mechanics to the prior described phase-field model are detailed in section 4.2.

As you will read in section 4.3, the phase-field approach is found to be rather computationally expensive, as well as depending heavily on tuning parameters, prompting efforts to reduce this by simplifying both fluid flow model, as well as thermal model. The reasoning on the proposed simplifications is shown in section 4.4. Results of the newly proposed models are shown in section 4.5. Efforts spent in stabilising them will be detailed in section 4.6. Finally in section 4.8 the conclusions concerning first-principle modelling and two-phase evaporative flows will be presented.

4.1. First-principle model scenario’s

As the VLM has a distinctly small height, and relatively large widths and lengths, a 2D flow approximation is argued to provide sufficient information on the flow, while simultaneously significantly reducing computation costs.

In order to be able to assess functionalities of the simulation methods, an abstract test is created. Instead of using real material properties and dimensions, normalised values are used, to be able to set up the most stable test environment. The properties and dimensions are denoted in table 4.1 and 4.2.
4. First-principle based model studies

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapour</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg m^{-3}]</td>
<td>$\rho_l = 1$</td>
<td>$\rho_v = \rho_l 10^{-n}$</td>
</tr>
<tr>
<td>Viscosity [Pa s]</td>
<td>$\mu_l = 1$</td>
<td>$\mu_v = \mu_l 10^{-1}$</td>
</tr>
<tr>
<td>Conductivity [W K^{-1} m^{-1}]</td>
<td>$\kappa_l = 1$</td>
<td>$\kappa_v = \kappa_l 10^{-1}$</td>
</tr>
<tr>
<td>Specific isobaric heat [J kg^{-1} K^{-1}]</td>
<td>$c_{p,l} = 1$</td>
<td>$c_{p,v} = c_{p,l}2^{-1}$</td>
</tr>
</tbody>
</table>

Table 4.1: Normalised liquid and scaled vapour properties.

Note that the vapour densities in table 4.1 are scaled to the power of $n$, allowing for an easy shift of densities ranging from identical to liquid ($n = 0$), to a similar difference as real liquid and vapour ($n = 3$). Furthermore, latent heat is chosen to be $10$ [J kg^{-1}], saturation temperature as $1$[K], and in the case of the Reynolds equation, the width of the phase transfer as $0.1$[K], and the standard deviation for the latent heat as $0.05$[K].

The scaled dimensions in table 4.2 refer to the available fluid domain, shown in from a top-down perspective in figure 4.1. Fluid flows into the system from the left (at minimal $x_1$), over the full width of the system. Outlet boundary conditions are applied at the right of the figure, over the full width. Side-walls are applied as appropriate boundaries, as shown in the figure as the top and bottom boundary, at minimum and maximum $x_2$ values.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width of system [m]</td>
<td>$W = 0.5$</td>
</tr>
<tr>
<td>Length of system [m]</td>
<td>$L = 1$</td>
</tr>
<tr>
<td>Height of system [m]</td>
<td>$H = 1$</td>
</tr>
</tbody>
</table>

Table 4.2: Normalised system dimensions.

Figure 4.1: The abstract model in COMSOL.

Next to the abstract model, a realistic model is created. This model uses both a realistically dimensioned VLM, as well as realistic material properties. Property values are shown in table 4.3, while the system dimensions are shown in table 4.4. Figure 4.2 shows the layout as used for this scenario. Note the absence of the nozzle, when compared to figure 2.1, as the nozzle will not be modelled using the same fluid equation, but rather as either a fixed pressure boundary conditions, or one dependent on the mass flow, using the ideal rocket theory (see equation 2.34). This boundary condition is applied at the far right of the figure, at maximum $x_1$ values, over the full width of the system. The inlet condition is located on the far left of the system (minimal $x_1$ value), and is applied over the width of the thin inlet section. Side-walls are applied elsewhere.

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapour</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg m^{-3}]</td>
<td>$\rho_l = 10^3$</td>
<td>$\rho_v = \rho_l 10^{-4}$</td>
</tr>
<tr>
<td>Viscosity [Pa s]</td>
<td>$\mu_l = 10^{-4}$</td>
<td>$\mu_v = 2 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>Conductivity [W K^{-1} m^{-1}]</td>
<td>$\kappa_l = 0.6$</td>
<td>$\kappa_v = 0.03$</td>
</tr>
<tr>
<td>Specific isobaric heat [J kg^{-1} K^{-1}]</td>
<td>$c_{p,l} = 4.2 \cdot 10^3$</td>
<td>$c_{p,v} = 2 \cdot 10^4$</td>
</tr>
</tbody>
</table>

Table 4.3: Realistic liquid and vapour properties. Latent heat is set up as $2.2 \cdot 10^6$ [J kg^{-1}]

In the case of the Reynolds equation (see section 4.4), the width of the phase transfer is defined as $3.5$[K], and the standard deviation for the latent heat as $1.75$[K].
Table 4.4: Realistic VLM system dimensions.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Width of system [mm]</td>
<td>$W = 3.0$</td>
</tr>
<tr>
<td>Length of heater [mm]</td>
<td>$L = 9.0$</td>
</tr>
<tr>
<td>Width of inlet section [mm]</td>
<td>$W = 0.4$</td>
</tr>
<tr>
<td>Length of inlet section [mm]</td>
<td>$L = 4$</td>
</tr>
<tr>
<td>Length of divergent section [mm]</td>
<td>$L = 2$</td>
</tr>
<tr>
<td>General Height of system [mm]</td>
<td>$L = 0.15$</td>
</tr>
</tbody>
</table>

Figure 4.2: The realistic model in COMSOL

4.2. COMSOL PHASE-FIELD APPROACH

This section will deal with the theory of the fluid-mechanics, heat transfer and phase-transfer equations, and how they are applied to the phase-field modelling method. First the application of the conservation of mass and momentum in thin-film flows is detailed, while interface mechanics are next. Finally heat transfer and phase-transfer equations are detailed, and their application will be highlighted.

4.2.1. CONSERVATION OF MOMENTUM AND MASS

The applied fluid mechanics model for the phase-field approach is the Navier-Stokes equation, as introduced in section 2.1.1. Similar to the prior explanation, the approach is to use a constant density for the liquid, and a variable density for the vapour based on the ideal gas law, equation 2.23. The momentum and mass conservation laws (equations 2.1 and 2.5) are repeated below for convenience, indicating, in order of appearance, momentum continuity and mass continuity.

$$\frac{\partial (\rho \mathbf{u}_3)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_3 \otimes \mathbf{u}_3 + p \mathbf{I}) = \mu \nabla^2 \mathbf{u}_3 + \rho g$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}_3) = 0$$

As the simulations are performed in a 2D planar model, the largest contributions to the momentum equation (namely the pressure drop due to viscous friction between fluid and top and bottom walls) is omitted in this 2D Navier-Stokes equation. This is therefore added as a body force, using equation 2.10:

$$\mathbf{u}_2 = -\nabla p \cdot \frac{H^2}{12\mu}$$

This entails a new momentum equation, for a 2D system with known and constant distance between the two out-of-plane bordering walls: equation 4.1.

$$\frac{\partial (\rho \mathbf{u}_2)}{\partial t} + \nabla \cdot (\rho \mathbf{u}_2 \otimes \mathbf{u}_2 + p \mathbf{I}) = \mu \nabla^2 \mathbf{u}_2 + \frac{12\rho H^2}{H^2} \mathbf{u}_2$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}_2) = 0$$

Prior work by among others [43] have re-introduced inertial effects in the Reynolds equation. However, as far as is know to the author of this thesis, none have so far also included the in-plane viscosity terms $\mu \nabla^2 \mathbf{u}_2$. 
This is probably in part due to application where the thin-film flow systems are used, as examples such as bearing and lubrication systems have negligible in-plane stresses.

The current design by [8] has however included flow-disrupting pillars, whereby the in-plane viscous stresses with these object become very much important again. Consequently the necessity to account for such effects results in a novel planar flow mechanics equation 4.1.

Note that in the latter part of equation 4.1 $u_1 \frac{\partial u}{\partial x_1}$ an implicit assumption concerning the velocity profile in the height dimension $(\partial_3)$ is posed, of a parabolic velocity profile. As inertia effects become more important, this profile might no longer be as clearly identifiable, and care should be taken in using this assumption. In appendix E a model-based investigation of the effect of accounting for this pressure drop is provided.

Though compression effects are seemingly not taken into account in the momentum equation, the vapour is able to change in density due to local changes in pressure. Therefore special care will have to be placed in the post-processing analysis of the local speeds. If these exceed $\nu > 0.3 \cdot u_{\text{sound}}$, compressibility effects will definitely have to be accounted for [17, 18]. As this is expected to occur in the nozzle section of the VLM, this section will not be modelled using flow equation 4.1.

4.2.2. FINDING THE INTERFACE

As suggested by [52] the calculation of the interface position is referred to as ‘direct numerical simulation of the interface motion’. As shown in section 2.3.4 the computation of the interface location is important for micro-fluid multiple-phase flows. This is either done by tracking it’s movement via a specific function, or via a marker function that defines the interface by means of a marker variable such as $\alpha$, with values of 0 and 1 indicating for instance liquid and vapour phase respectively, and intermediate values indicating an interface.

Initially phase-field method is used, explained in greater detail in appendix B. Suffice to say that the Cahn-Hilliard equation used as a basis employs a marker function and variable, that varies between -1 and 1, where the outer values indicate a pure substance, and intermediate values indicate an interface.

The Cahn-Hilliard equation itself shows on the left side the local change and advection of the marker, while on the right side a ‘driving’ function of $\Psi$ is shown:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \chi \omega \nabla \Psi$$

(4.3)

The ‘driving’ function included in equation 4.3 is based on the chemical potential $\Psi$. This potential causes the two phases to resist intermingling, and is defined as:

$$\Psi = \omega - \nabla^2 \cdot \frac{\partial \phi}{\partial x} \frac{\partial (\phi^2 - 1)}{\partial x}$$

(4.4)

The terms $\chi$, $\omega$ and $\zeta$ introduced in these equations need to be tuned. The variable $\chi$ dictates the mobility of the interface: larger values dampen the movement, but ensure that the interface remains compact, while lower values allow for a more fluid interface, but potentially allow it to be diffused. By default, this value is 1. Initial tests showed that default $\chi$ values did indeed produce significantly smeared interfaces. Setting its value to 25 was experimentally determined to provide be required to ensure a non-diffused interface. The initial interface width $\zeta$ was left at default settings.

The variable $\omega$ refers to the mixing density, a function of the surface tension and interface thickness $\zeta$. By default, the value of $\zeta$ is half the maximum size of the elements used. This value is maintained.

4.2.3. INTERFACE EQUATIONS

In multi-phase flow with phase transfer an exception to the rules concerning the continuity of the velocity field is made. At the phase boundary due to the shift in density and the evaporation mass flux, the fluid velocities at both sides of the interface can be expressed as in equation 4.5.

$$\mathbf{n} \cdot \rho_V \mathbf{u}_V = G_{\text{evap}} \left(1 - \frac{\rho_V}{\rho_L}\right) + (\mathbf{n} \cdot \rho_V \mathbf{u}_L)$$

(4.5)
Here $G_{\text{evap}}$ refers to the evaporation mass flux and $\mathbf{n}$ to the normal unit vector with respect to the interface. As seen in equation 4.5, the velocity field is only continuous over the interface in the case of equal densities and/or zero mass transfer across the interface. Concerning evaporative flows of water in sub-critical conditions, the densities of liquid and gas are never equal, and therefore given a mass evaporation, the velocity field is expected to be discontinuous.

Having previously concluded in section 2.3.4 that the surface tension is the main force on the interface, it is modelled using the chemical potential (see equation 4.4). This force is introduced in the momentum balance using the said chemical potential multiplied by the phase field spatial divergence, as seen in equation 4.6:

$$
\rho \frac{\partial \mathbf{u}_2}{\partial t} + \rho (\mathbf{u}_2 \cdot \nabla) \mathbf{u}_2 = \mu (\nabla^2 \mathbf{u}_2) - \nabla p + \nabla_2 \mathbf{u}_2 \frac{12\mu}{H^2} + \Psi \nabla \phi
$$

The continuity equation 4.7 applied to the system is adjusted to take into account the possibility of mass transfer, by not setting the divergence of the velocity field to zero, but equating it to the mass flux over the interface times the $\delta$ function that ensures that the continuity can only be non-zero at the interface. The $\delta$ function is a smoothed representation of the interface between the two phases. It is always zero, except for the interface region. For a more encompassing explanation of the $\delta$-function, please see appendix B.

$$
\nabla \cdot \mathbf{u}_2 = G_{\text{evap}} \delta \left( \frac{1}{\rho_V} - \frac{1}{\rho_L} \right)
$$

The right hand side of equation 4.7 is implemented as a variable in COMSOL. If vapour and liquid densities are held equal and constant, the result of equation 4.7 is once again a solenoidal velocity field.

**Heat transfer**

As fluids are the subject of investigation, heat transfer can be captured by the term convection and radiation. In this instance the Navier-Stokes heat transport equation will be used: equation 2.15.

Concerning the implementation of latent heat: when a non-zero latent heat is present, the process of mass transfer from one phase to the next will also dictate a shift of energy. This is implemented in the energy flux equation 4.8.

$$
\rho c_p \frac{\partial T}{\partial t} + \rho c_p \mathbf{u}_2 \cdot \nabla T = -\nabla \cdot (\kappa \nabla T) + h(T_s - T) - H G_{\text{evap}} \delta e_{1L}
$$

The section of $H G_{\text{evap}} \delta e_{1L}$ indicates the rate of energy transfer due to the mass flux of evaporation in the 2D system of height $H$, times the latent heat of evaporation per kg. This approach of course implies some knowledge on the speed of mass transfer from liquid phase to vapour phase.

Concerning the properties involved: apparent from equation 4.8 are the important parameters: conductivity of the fluid, density of the fluid, isobaric specific heat and latent heat of vaporisation.

The average property for any volume element in the simulation is determined by the volume fraction of each phase occupying that element, using equation 4.9, which is in this case either liquid or vapour, except for the transition region between the two pure phases.

$$
b = \alpha b_V + (1 - \alpha) b_L
$$

Here $\alpha$ is the phase indicator, varying between 0 for the liquid phase, and 1 for the vapour phase.

**Evaporation mass rate**

COMSOL uses a relatively simple evaporation method, shown in equation 4.10:

$$
G_{\text{evap}} = C \rho_L \frac{T - T_{\text{sat}}}{T_{\text{sat}}}
$$

The factor $C [\text{ms}^{-1}]$ controls the rate of evaporation mass flux given a temperature $T$, and consequently influences evaporation behaviour to a large extent. Therefore setting this factor $C$ too low results in a drift of
the phase-boundary away from the saturation temperature. As shown in appendix B in section B.2, the evaporation rate setting of $C = 1.5$ approximates theory presented by Tanasawa at pressure conditions of 0.5[bar], while a factor of $C = 11.5$ approximates this theory at pressure conditions of 5.5[bar]. These values will be used in this thesis. For more background information on evaporation at interfaces, see appendix B in section B.2.

IMPLEMENTATION OF THE MASS TRANSFER OVER THE INTERFACE

The mass transfer is applied using a weak contribution over the entire design domain to account for both phase transfer in the phase-field equation and mass transfer in the mass continuity equation. It is evaluated in weak form in COMSOL, as in equation 4.11:

$$\text{test(}{\psi}\text{)} \cdot \left( -G_{\text{evap}} \delta \left( \frac{\nu_d}{\rho_V} + \frac{1 - \nu_d}{\rho_L} \right) \right) + \text{test(}{p}\text{)} \cdot \left( -G_{\text{evap}} \delta \left( \frac{1}{\rho_V} - \frac{1}{\rho_L} \right) \right) = 0 \quad (4.11)$$

The first part indicates a test function of the $\psi$ variable embedded in the phase field variable $\phi$ (see equation 4.4). By multiplying the test variable with $-G_{\text{evap}} \delta \left( \frac{\nu_d}{\rho_V} + \frac{1 - \nu_d}{\rho_L} \right)$ the expression forces $\psi$ to switch sign and change its magnitude for a mass transfer from liquid to vapour, and similarly for the test variable for pressure $p$. Please see section B.2 for a broader explanation of the phase-field application. Equation 4.11 ensures that any phase change mass transfer will relate to a shift of the phase field.

4.3. PHASE-FIELD RESULTS

Using the approach detailed in the prior section, the phase-field model is applied to the scenarios described in section 4.1.

4.3.1. ABSTRACT MODEL SIMULATIONS

Unfortunately, the abstract model fails to run using the phase-field method. The system reports an inability to find converged first time step with heat transfer. Despite considerable effort, the error was not isolated, and no results were created.

4.3.2. REAL SYSTEM SIMULATIONS

The phase-field tests are performed on the realistic model, of dimensions listed in table 4.4 and fluid properties listed in table 4.3.

<table>
<thead>
<tr>
<th>Case number</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber pressure</td>
<td>0.5[bar]</td>
<td>5.5[bar]</td>
</tr>
<tr>
<td>Mass flow</td>
<td>0.12[mg]</td>
<td>0.12[mg]</td>
</tr>
<tr>
<td>$T_{\text{sat}}$</td>
<td>373[K]</td>
<td>429[K]</td>
</tr>
<tr>
<td>Wall temperatures</td>
<td>400 to 500[K]</td>
<td>450 to 550[K]</td>
</tr>
<tr>
<td>$C$</td>
<td>1.5[m s$^{-1}$]</td>
<td>11.5[m s$^{-1}$]</td>
</tr>
</tbody>
</table>

Table 4.5: Test set-up CFD tests

For fluid properties used, please see table 4.3. Note that in the phase-field simulations, the Nusselt number is set to 6, as the system calculates the heat transfer to single-phase systems separated by an interface, and as such needs no extra heat transfer correlations.

EXTRA SIMULATION CONDITIONS

Note that simulations were all assessed with the inlet-channel section at saturation temperature, resulting in a fully saturated liquid. As the single-phase heating process is relatively straightforward, and as evidenced by the analytical models, very fast, it was deemed not necessary to compute this process, simplifying the involved physics for the evaporative process in the phase-field method.
Furthermore instead of inlet and outlet pressure conditions, as per real mode of operation, a mass-flow inlet condition and reference outlet pressure are used, to simplify simulations. This method can possibly lead to reduced oscillatory behaviour, as the incompressible liquid in the entrance region is forced on due to the mass-flow inlet condition (as was noted in section 2.4).

To compare the results obtained in the correlated analytical models to the CFD analysis, similar test are conducted. The wall temperatures selected for these tests are 400, 425, 450, 475, 500, 525 and 550 [K], and an overview of these results is bundled in figure 4.3.

\[(a) \ p_{in} = 0.5\text{[bar]}, T_{w} = 400\text{[K]}\]
\[(b) \ p_{in} = 0.5\text{[bar]}, T_{w} = 425\text{[K]}\]
\[(c) \ p_{in} = 5.5\text{[bar]}, T_{w} = 500\text{[K]}\]
\[(d) \ p_{in} = 5.5\text{[bar]}, T_{w} = 525\text{[K]}\]

Figure 4.3: The temperature field shown with colour range (in [K]), with the interface location denoted with the marked grey section.

**0.5[bar] Test**

The test shown in figure 4.3a was conducted with a wall superheat value of 45.7[K] (absolute wall temperature of 400[K]). Consequently, it was expected that the energy influx into the system would be sufficient for the fluid to be able to evaporate, given the inflow mass velocity computed using the balance model of just 0.12[\text{mgs}^{-1}].

This is indeed visible in the simulation results showed in figure 4.3a. The interface, or liquid to vapour transition region (marked with a grey line in the plot), does not move much from its initial position.

As the liquid entering the system is already at saturation temperature, and the inlet section is subjected to a wall temperature of just the saturation temperature, it is curious to see that the interface has remained at the inlet section: this indicates that the required heat energy enters the system in the vapour section, and must flow through the fluid layer to the interface, where the energy is used to evaporate the liquid.

Similarly, a wall temperature of 425[K] shows a quickly established equilibrium, visible in figure 4.3b. The regression of the interface region back into the inlet channel is much more pronounced in this case, as it sits comfortably in the inlet section. This indicates that despite a very thin layer of fluid present, and vapour-phase thermal conductivity obstructing heat conduction (as opposed to the much higher conductivity of liquid), sufficient amounts of heat are transport against the fluid-flow direction.

The result of this successful evaporation at a pressure of 0.5[bar] correlates to the similar results obtained using the analytical models (see figure 3.14).

Note that the analytical tests use a uniform wall temperature, also in the inlet section. As such, the system is simulated using the analytical model already is in the process of adding heat energy to evaporate the system in he inlet section. Note that despite that, evaporation is not complete in the inlet section of the system for
the 430[K], 0.5[bar] case. The neglecting of longitudinal heat transport in the analytical case might be debit to that.

5.5 [BAR] TESTS

Case two of the CFD tests, as suggested in table 4.5, uses a pressure of 5.5[bar], and mass flow rate of 1.2[mgs\(^{-1}\)]. As the saturation temperature at a fluid pressure of 5.5[bar] is 429[K], the first viable test where evaporation can be expected is the 450[K] wall temperature test.

The wall temperature surplus of just 23[K] is not sufficient to maintain a constant evaporation front, similar to results described using the analytical model where this case is shown in figure 3.23. As such a similar liquid-superheat result as shown in figure 4.3c is seen, though now heated to the wall temperature of 450[K].

However increasingly high wall temperatures, even the case with 71[K] wall temperature superheat compared to the saturation temperature \((T_w = 500[K])\) resulted in incomplete evaporation, as seen in figure 4.3c. This contradicts with the expected results of the analytical calculations, where a wall temperature of 455[K] was deemed sufficient to evaporate the full fluid in the 5.5[bar] case, as seen in figure 3.23.

When the wall temperature is raised to 525[K], the wall temperature surplus of 96[K] is seen in figure 4.3d to be sufficient to maintain a constant evaporation front. Alike the 0.5[bar] simulations, the results show that all liquid is evaporated immediately upon entering the heater section with superheated wall temperatures, though in this case the front does not recede into the inlet channel.

PRESSURE BOUNDARY CONDITIONS

So far, the systems have been investigated using mass-flow boundary conditions. When instead of mass-flow, steady-state pressure boundary conditions are used, the liquid and vapour front is provided more freedom to move around. Unfortunately this requires so much more computation time, that it was infeasible to compute a full simulation of reasonable simulated time on the computer used.

4.3.3. COMPUTATION TIME

The computation time between solutions shown in figure 4.3 varies significantly. Simulations where the interface remains located at the border between inlet-section and divergent section are usually calculated in 10 to 20 minutes, varying with mesh size.

However, simulations such as those shown in figures 4.3a and 4.3c, where the interface is advected across the fluid domain, tend to take up to 4.5 hours for the first 0.2 seconds, until the interface has moved beyond the limit of the domain, and COMSOL can increase the time-steps of the calculation. The computer used for the computations contains 8 GB of RAM and a 2.9 GHz i5 2-core Intel processor from 2012. Both cores are assigned to the computation.

4.3.4. REVIEW OF THE PHASE-FIELD METHOD

The presented results of the COMSOL phase-field method show that given only a slim superheat of 50 K, the system is able to evaporate the full fluid easily, for a 0.5[bar] chamber pressure and mass influx of 0.12[mgs\(^{-1}\)]. Moreover, the system shows a tendency to have a full evaporation of liquid at the border between the inlet section and the divergent heater section. It would appear that the heat conducted to the interface is in this instance large enough to maintain a constant (steady-state) boundary position.

However, as the simulation is rather sensitive to the tuning parameters mentioned in the previous section, validation experiments will be required. In line with this assessment, the experiment by [16] showed snake flow, which was unfortunately not repeatable using the phase-field method. Secondly, the small droplet formation observed by the same authors, or the oscillating flow boiling phenomenon observed by [31], were similarly not seen.

Furthermore, though simulations are stable, it is clear that the restriction stipulating that evaporation may only occur at interfaces, prevents sufficient evaporative mass flux despite very high superheat temperatures of both liquid and vapour. Reported superheat in the liquid of 71[K] for the 5.5[bar] case has so far not been
observed in real experiments according to the authors knowledge. A superheat of this magnitude would require a local vapour embryo to be created due to present surface roughness effects [32], which is rendered impossible due to the method of phase-field simulation. Due to the very high computation costs of partially evaporated systems, the phase-field approach appears not to be very practical for use in numerical optimisation routines.

Finally, it should be noted that the influx of heat into the system assumes pure fluids at either side of the interface. In reality, annular flows and mist flows have been reported, changing the heat flux coefficients drastically. This is however a draw-back of any 2D model.

4.4. SIMPLIFICATIONS OF PHYSICS

The prior approach to two-phase simulations provides a sample of the available approaches, all depending on the core principles as outlined before: the interface must be tracked, inducing extra computational effort on the computation.

However, if the added pressure-modifying behaviour of the surface-tension can be predicted regardless of the fluid-motion present, this will reduce computational effort.

4.4.1. SURFACE TENSION SIMPLIFICATION

By setting up the same assumptions as prior for the Reynolds equations (properties are assumed constant over a vertical column of material), the surface tension that results from a curvature in the vertical direction must also be constant. In effect, this assumption has been implicitly made in the prior phase-field simulations.

Based on the work of [53], hydrophilicity angles can be estimated if the thickness of the layer of SiO$_2$ grown on the Si base layer is known. Based on the work of [54], this layer can safely be assumed to have grown to more than 30 Angstroms due to testing occurring prior to launch, resulting in a fully hydrophilic layer. This then entails an equilibrium contact angle of 0 deg, returning a radius of the curvature of half the height of the heater in the vertical direction, and of approximately half the width in the horizontal direction.

The pressure difference induced by this curvature can be calculated using equation 4.12, as introduced by [24], where $R$ represents the local curvature radius.

$$\Delta p_\sigma = \frac{\sigma}{R} \quad (4.12)$$

Note that equation 4.12 is different from equation 2.44, as the latter equation takes into account a curvature over two dimensions simultaneously, and the current equation only does so for a single dimension at the time. The curvature over the width of the system is a factor of 20 larger than that over the height of the system. Using a surface tension coefficient $\sigma = 0.058$[N/m], a width of $W = 3$[mm] and a height of $H = 0.15$[mm], the extra pressure generated by the width of the flow is approximately 39[Pa], while the pressure generated by the height is approximately 0.79[kPa]. As such the in-plane surface tension is expected to be negligible, and for now disregarded in the computation.

Furthermore, as the out-of-plane pressure difference due to surface tension is uniform over any interface, as it is dictated nearly exclusively by the vertical curvature, the difference between phases must be a constant pressure. This effect on properties can therefore be pre-computed, reducing the need for the application of this surface-tension force on the fluid.

Consequently, there is no need for the definition of a phase-boundary based on the pressure field, as no significant unknown forces are acting on it.

4.4.2. EVAPORATION REGION SIMPLIFICATION

The in section 4.2 highlighted theory on evaporation speed relies on a temperature gradient, and requires an exactly defined phase-boundary.
Using the introduced surface tension simplification, the interface no longer needs to be defined to apply surface tension forces. A simplification for the evaporation system is now in order, to be able to fully simplify the two-phase simulation.

If now instead of evaporation occurring at a single saturation temperature, evaporation would occur over a temperature range like ideally mixed substances, a measure for mass transfer over an interface is no longer required.

First, the range over which the phase variable changes is determined as $\Delta T$, which encompasses the section where 99% of the shift of property is completed. This requires a factor of $\omega = \Delta T / (2\pi)$. The method of shifting using a hyperbolic-tangent function is shown in equation 4.13.

$$X = \left[ \frac{T - T_{sat}}{\omega} \right]$$

$$\alpha = \frac{1}{2} \left( 1 + \frac{e^{2X} - 1}{e^{2X} + 1} \right)$$  \hspace{1cm} (4.13)

In COMSOL a similar equation using a 6th order polynomial called the 'FLC2HS' is used, that mimics the hyperbolic tangent behaviour, with the added benefit that outside of the intended shift range, the gradient is zero. Once the phase variable has been determined, the local specific isobaric heat is computed, using equation 4.14.

$$c_p = c_{p,V} \alpha + c_{p,L}(1 - \alpha)$$  \hspace{1cm} (4.14)

Next to this application of specific heat, the latent heat needs to be accounted for. To do so, its contribution to the specific energy in the fluid is also smeared, using a Gaussian distribution:

$$\Delta e_{HL,\sigma}(T) = \frac{e_{HL}}{\sigma_{sd} \sqrt{2\pi}} \exp \left( -\frac{1}{2} \left( \frac{T - T_{sat}}{\sigma_{sd}} \right)^2 \right)$$  \hspace{1cm} (4.15)

Here $\sigma_{sd}$ represents the standard deviation for the Gaussian distribution.

Implementing this in a simple model relating fluid enthalpy to phase change, the two models are seen to differ little in the evaporation region, as is visible in figure 4.4.

![Figure 4.4: Smearing the evaporation region, (red and purple), versus pure evaporation (blue and yellow).](image)

In figure 4.4, the dotted lines denote the ‘phase-variables’. The yellow line indicates the ‘instantaneous’ shift of phase as temperature reaches the boiling point, from pure liquid to pure vapour, while the blue line shows the normalised enthalpy increase needed to allow this phase shift.
In contrast, the purple dotted line and red line show the phase-variable shift over a small temperature range, starting just below the boiling temperature, and continuing just beyond the boiling temperature. Similarly, the energy needed to ensure that phase shift occurs is distributed, resulting in a smoothed shift, improving computational stability.

Next to possibly improving computational stability, this method allows the phase border to be linked to a temperature gradient, reducing the need to define a phase border, and completing the goal set out at the binning of this subsection.

4.5. Initial Reynolds-Model Results

Observing in the property-list for the abstract simulation set-up (see table 4.1), initial simulations are set with a density changing factor of $n = 2$, or the density of the vapour-phase is one-hundredth of that of the liquid. The simulation remains stable, and results are shown in figure 4.5. Note that due to the large effect of the latent heat in the region of evaporation, a relatively large section of the heater is shown with near-constant temperature, to pass the range where the latent heat is added, seen in figure 4.5a. Similarly, a smooth decrease in density of the liquid is seen in figure 4.5b.

However, when the same model is applied to a simulation using more realistic density properties for the vapour (a factor of 1000 of the density of the liquid), most simulations fail quickly with exceedingly large (or very negative) temperature and pressure results. An example of such a result is shown in figure 4.6. As the expected pressure drop values lie in the order of $10^1$ to $10^3$[Pa], the reported pressure drops during error of $10^{140}$[Pa] or more are the result of numerical errors.

In fact, comparing the last stored reasonable density distribution shown in figure 4.6a to the final crash-report density plot of figure 4.6b, two things are clearly lost:

1. The relatively smooth shape (wide curve) of the transition regime spanning the width of the heater
2. The transition width between fully liquid and fully evaporated fluid

The first loss may be written off as a series of bubble explosions, alike those observed in the various pa-
pers shown in section B. However, the very sharp density transition between fully vapour and fully liquid begs some critical notion, as any temperature gradient over those sections would encourage heat flux from hot vapour to cooler liquid. However, the temperature figures for the result ranged between $1 \times 10^{140}$ [K] to $-1 \times 10^{120}$ [K], clearly in error, as the inlet temperature was 0 [K], and the wall temperature 2[K].

Of note is too a strange occurrence in what at first seems still a stable and reasonable simulation result, at figure 4.6a: the phase field is curved. The out-of-plane wall temperatures are set to be uniform, while the in-plane walls (side boundaries) are simply isolated, and allow no heat transfer. As such, no difference in initial heat flux to the fluid is expected, yet it still develops smoothed curves in the temperature field.

4.6. ANALYSIS OF MODEL INSTABILITIES

When reviewing the instabilities, both the underlying physics as well as numerical stability are analysed. First the physics will be covered, and next the numerical stability criterion of the Peclet number is studied.

4.6.1. PHYSICS OF THE DIFFICULTIES

When viewing boiling from a macroscopic level, the process seems mild. But as assessed by among others [24, 32, 37] small dimension systems can experience large pressure fluctuations and flow-reversals. As such, the process itself can be considered explosive.

The time-dependent test shown in figure 4.7 to analyse this phenomenon is conducted using a hypothetical volume element of thickness $H$, and unit length and width, prior to heating filled with liquid at a temperature below saturation temperature, and heated using the same analytical equations as in section 3.5.2, equation 2.13.

Consequently, using the distributed latent heat and specific energy from equations 4.15 and 4.14, and the density calculated using the phase-variable ratio of liquid and vapour (see equation 4.13), the heat equation 2.15, where the fluid velocity (and therefore convection effects) are discounted.

Figure 4.7b show the density-time evolution of an arbitrary element heated at realistic heat fluxes (based on the analytic model of chapter 3), while figure 4.7a shows the temperature evolution of the same volume element.

Both density and temperature are shown to smoothly change from liquid to vapour densities, for unrealistically high vapour densities of $\rho_V = 100$ [kgm$^{-3}$], but increasingly fast for very low densities observed in VLM’s during initial start-up. Especially the case with a pressure of just 100[Pa] or $1 \times 10^{-3}$[bar] should be noted, as this is a scenario occurring during start-up: liquid rushing into the heater after opening the feed-valve, encountering a very low pressure system.

![Figure 4.7: Volume element heating, observing temperature (a) and density (b).](image)

The increasingly fast heating seen in figure 4.7 is due to the lower density vapour tests having consequently a lower volumetric heat capacity (see figure 4.8b), in contrast to the smooth specific energy capacity, as in
4.6. **ANALYSIS OF MODEL INSTABILITIES**

(a) The specific energy capacity of the fluid

(b) The volumetric energy capacity of the fluid per unit of temperature

Figure 4.8: The Specific energy capacity (a), and volumetric energy capacity (b), per unit of temperature

The reduction of heat capacity of the volume element over time leads to an increasingly fast heating process. In other words: though the initial phase-transfer process is smooth, its smoothness is halted as enough heat is transported into the volume element to ensure complete evaporation.

This increasingly fast temperature rise also influences the amount of fluid able to fit in the element. As the liquid initially occupying the vapour element had a higher density, this mass will have to be removed, creating a pressure differential.

### 4.6.2. **TEMPERATURE AND PRESSURE FIELD OSCILLATIONS**

During simulations often wave-like oscillations are observed in the temperature and pressure fields. At times, these will dampen out. However, they do not always resolve correctly, leading to local extreme temperature and pressure values, and loss of convergence in the simulation.

These oscillations are known to occur in any transport problem where convection plays a larger role than diffusion. Using for instance equation 4.16, scaling factors $\beta$ and $\nu$ are the scaling factors for convection and diffusion respectively.

\[
\frac{\partial b}{\partial t} + \nu \nabla b = \nabla \cdot (\beta \nabla b) + F \tag{4.16}
\]

The Peclet number is calculated as in equation 4.17. When the Peclet number is more than 1, oscillations such as those mentioned are likely to occur. Note that $L_{\text{elem}}$ is the characteristic element length used in the mesh for the numerical calculation.

\[
Pe = \frac{L_{\text{elem}} \beta}{2\nu} \tag{4.17}
\]

For heat transfer, factor $\nu$ can be understood to be the local velocity times density and specific isobaric heat, while $\beta$ is the conductivity of the fluid. The Reynolds equation, as shown in equation 2.9, has solely ‘conductive’ components, and as such should have a Peclet number of 0.

The heat transfer equation however does not have a Peclet number of zero, leading to possible issues. Observing equation 2.15, it is apparent that if the velocity becomes markedly large, the Peclet number grows beyond one.

To remedy oscillatory effects high-Peclet number equations, COMSOL offers some stabilisation options:

1. Inconsistent stabilisation
2. Consistent stabilisation
Inconsistent stabilisation adds a diffusive component to the equation \(4.16\), allowing \(\nu\) to become \(\nu + \nu_{\text{stab}}\). For a heat transfer equation, it ramps up conductivity of a fluid:

\[
v_{\text{stab}} = \delta_{\text{stab}} L_{\text{elem}} \nu
\]  

(4.18)

Here \(\delta\) is a tuning parameter. The effective Peclet number becomes:

\[
Pe = \frac{L_{\text{elem}} \nu}{2\nu + 2\delta_{\text{stab}} L_{\text{elem}} \nu} 
\]  

(4.19)

This method is generally effective at reducing simulation instabilities, though it arbitrarily adds the stabilising diffusion component, and does not temper its approach based on a possibly already well-operating simulation.

In contrast with this, the second option referred to as ‘consistent stabilisation,’ provides less extra diffusion the closer the solution gets to the exact solution [55]. COMSOL offers the two options of firstly streamline stabilisation, adding a diffusive component only in the stream-wise direction (along the flow vector), and cross-wind diffusion, which as the name suggests adds diffusive effects perpendicular to the flow directions. The latter option is said to also reduce numerical oscillations, on of the issues encountered.

COMSOL [55] suggests the use of consistent stabilisation as it is said to converge quicker to the exact solution for decreasing mesh sizes than the inconsistent stabilisation technique.

These consistent stabilisation techniques are as-default active in the COMSOL solver for physics that support them, though tuning might allow for better results. They are however not available in the thin-film physics model.

### 4.6.3. Applied Stabilisation Methods

Even though the Reynolds equation has a Peclet number of 0, oscillatory behaviour appears to arise also from the pressure calculations. Indeed, after allowing full inconsistent and consistent stabilisation in the heat transfer equations, still oscillations were present in the simulations, and often the simulation would fail to run for the indicated time. Therefore stabilisation methods are applied using the dilated species physics and the basic Navier-Stokes physics interfaces, for the pressure calculations.

#### Diluted Species Physics

Firstly, the physics model for ‘diluted species’ is (ab)used to enable modelling of a pressure distribution, while allowing the system to enable consistent stabilisation. The basic equations governing the ‘diluted species’ physics is shown in equation \(4.20\).

\[
\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i 
\]  

(4.20)

Here \(c_i\) [molm\(^{-3}\)] represents a dissolved species, \(D_i\) [m\(^2\)s\(^{-1}\)] the coefficient of diffusion, and \(R_i\) [molm\(^{-3}\)s\(^{-1}\)] the reaction speed. Though the units will seem odd, equation \(2.9\) can be imagined to fit into equation \(4.20\), when the convective elements are set to zero, and the local time-change of the species are eliminated through a weak-form expression:

\[
\nabla \cdot (-D_i \nabla c_i) = R_i 
\]  

(4.21)

Now \(-D_i\) is recognised as \(\left[ \frac{\mu H^3}{12 \mu} \right]\), while the reactive component \(R_i\) is recognised as \(H \frac{\partial p}{\partial x_i}\).

The mass influx boundary condition is expressed using equation \(2.10\), and the mass mass flow equation with the cross-sectional area \(A_{cs}\), and the velocity perpendicular to the cross section \(u_i\):

\[
\dot{m} = u_i \rho A_{cs} = -\frac{\partial p}{\partial x_i} \frac{H^2}{12 \mu} \rho A_{cs} 
\]  

(4.22)
Rewriting equation 4.22 to extract the pressure gradient creates:

\[ \frac{\partial p}{\partial x_i} = -\frac{12\eta\mu}{H^2 \rho \Lambda_{cs}} \] (4.23)

Which now relates the pressure gradient to a mass flux, given system dimensions. This allows the creation of not just a zero reference pressure conditions, but also a mass-flux inflow condition.

**Diluted species results**

To assess the viability of the method, 2D tests using the Reynolds equation are performed, using scaled properties defined as in table 4.1. Unfortunately, the diluted species approach appears to yield no perceptible improvements concerning stability. Both equations yield stable simulation results for the case where the \('vapour\'-density is increased to 10[kgm^{-3}], using a free-triangular mesh, with a maximum characteristic length of 0.01[m], resulting in a simulation with approximately 50000 DOF’s.

Considering that the stabilisation attempts to increase the conductive component \(D_t\) for the inconsistent stabilisation (see section 4.6.2), this is in effect similar to applying the simulation with more height, or indeed a larger density or lower viscosity, as is apparent from the terms dictating \('conduction\': \[ \rho H^3 \frac{\partial \phi}{\partial x_i} \].

The differences in simulation results between the diluted species result and the original Reynolds-equation result are indistinguishable. Similarly the computation time is unaffected, both amounting to approximately 5.5 minutes for the diluted species runs, and 4.5 minutes for the thin-film physics simulations.

**4.7. Adjusted physics results**

As indicated in the beginning of chapter 2 in section 2.1.1, the Navier-Stokes equations are considered one of the basis of the fluidic calculations for laminar flows. As indicated by [55], the resolution of the Navier-Stokes equations requires consistent stabilisation according to the work of Babuska [56] and Brezzi [57]. Consequently, a large measure of stabilisation is applied to these elements in COMSOL. As the viscous friction forces generated by the in-plane boundaries is limited, and the pressure drop would be underestimated, equation 4.1 as introduced prior is used.

This approach consequently still requires the resolution of the more computationally involved Navier-Stokes equation, and is therefore not ideal to save computation time. However, as stabilisation techniques are already implemented, this might provide a better insight into the possibilities present for the Reynolds-equation application in two-phase flow studies, combined with the gradual phase-change implemented in the thermal equations.

**4.7.1. Navier-Stokes results**

This new method ensures that for all tested densities in the abstract model, the simulations are able to compute the result. The most realistic results, for a density difference of a factor of 2000, are shown in figure 4.9. Though the shown figures are created using simulations with a comparable mesh as those used previously for the diluted species approach and the Reynolds equation approach, this model will still successfully compute the steady-state condition with much less detailed meshes, reducing computation time from 6 minutes to about 1.5 minutes.

Note in figure 4.9a the higher temperature is located near the in-plane wall boundaries, as the fluid moves slowest due to friction, and pressure peaks in figure 4.9b near the wall at the evaporation region and outflow region.

Some pressure oscillations are still visible at the onset of the simulations, especially around corners. This is visible in figure 4.10, especially where the wall boundary conditions meet in and outflow conditions. These oscillations grow more severe in simulations with larger mesh-elements, but tend to dampen out after several small time-steps. The pressure plot shown is augmented with a height-function, indicating that the height-dimension is a function of the local pressure, to be able to more easily distinguish the pressures in the fluid.
4. FIRST-PRINCIPLE BASED MODEL STUDIES

(a) The temperature distribution in the fluid.  
(b) The pressure distribution in the fluid.

Figure 4.9: The plots for temperature and pressure distributions at steady state, with isotherms of 0.9, 1 and 1.1 indicated in grey lines.

4.7.2. REAL SYSTEM SIMULATIONS

No stable realistic simulation using just the Reynolds equation has been successfully implemented: COMSOL reports unsolvable errors.

Most promise is shown by the Navier-Stokes approach, showing reasonable stability in the simulation attempts of realistic scenario’s.

However immediately upon start-up of the simulation large oscillations in the pressure field will occur. Their magnitude remains limited, possibly due to the stabilisation terms embedded in the Navier-Stokes physics model of COMSOL, causing a damping of the pressure spikes. This renders a situation that is still far from an acceptable solution, as these oscillations do not only occur near the phase-interface, but occur throughout the whole design domain.

It is unclear whether these oscillations seen in figure 4.11 perpetuate from the corner-oscillations observed in the abstract case in figure 4.10, or if they originate in the interface. Next to the pressure oscillations, figure 4.11 also shows a seemingly random very large temperature oscillations, which at times shows a single volume element to have temperatures well below inflow and wall conditions.

The computation of this realistic scenario is costly, as the computation of $0.5 \, [\text{ms}]$ is executed in time-steps of approximately $1 \cdot 10^{-10} \, [\text{s}]$, for a mesh with nearly 40000 elements. This is due to a lack of possible acceleration of the computation, due to the oscillatory behaviour.
This chapter saw the application of the phase-field model, the two-phase evaporation model suggested by COMSOL (sections 4.2 and 4.3). While a ready-made simulation routine facilitates ease of implementation, the approach is not without downsides: though the results for lower pressure simulations are in accord with the correlated analytical models, the higher pressure and mass-flow cases show significantly higher wall temperature requirements to ensure complete evaporation.

Experiments investigated in chapter 2 show oscillatory flow and explosive boiling in micro-channels. None of these elements were observed in the phase-field simulation. The susceptibility to tuning parameters like mobility and initial interface thickness also requires further effort. Based on the findings presented in this chapter, it is concluded that the phase-field two-phase evaporative flow simulation is too sensitive to tuning parameters, to be used without increased tuning and validation efforts. Due to the relatively large computation time, especially in partially evaporated situations, the phase-field approach is also considered too computationally intensive to be considered for numerical topology optimisation algorithms.

To provide an alternative, a reduced model is proposed in section 4.4, based on the Reynolds equation and a smoothed continuous evaporation method.

Despite showing theoretical promise, this method provides no stable useful simulations, due to instabilities occurring when the densities of the phases differed too much (see section 4.5).

Reintroducing inertia terms, as well as accounting for in-plane viscosities, a novel planar fluid approach is created that holds potential to allow a more efficient numerical analysis of two-phase flows.

Applying the novel fluid mechanics equation, together with stabilisation techniques implemented by COMSOL for the Navier-Stokes physics, resulted in stable and fast simulations for density ratios of (as tested) 2000, sufficient for the VLM at hand. The speed at which the computations were performed also suggests a possible application in numerical optimisation.

However, continued effort in the stabilisation methods is required before the new two-phase simulation approach can be utilised in realistic simulations, as oscillations perpetuated throughout the flow-domain in the initial tests executed with realistic material properties.

The questions posed at the beginning of this chapter concerning the investigation in flow-boiling behaviour can therefore not be answered with the models presented here.
CONCLUSIONS AND RECOMMENDATIONS

The work that formed this thesis set out to efficiently model two-phase evaporative flows in micro-structures, and investigate possible design improvements. To do so, both analytical and numerically solved first-principle models have been presented.

5.1. CONCLUSIONS

Thanks to the analytical and first-principle-based models, new insights in both modelling approaches, as well as design strategies for VLM's have been formulated. This section will detail them separately, first the modelling insights, and secondly the design insights.

5.1.1. MODELLING

Using analytical models, covering both an energy-balance model, as well as 1D fluid flow models, expected system efficiencies, propellant efficiencies, minimal wall temperatures and a prediction of the average power distribution for the full range of operating conditions have been presented in chapter 3. The analytical approach has provided clear performance targets for the operation of the VLM. The modelling methods presented here provide a novel way of quickly assessing VLM designs, allowing for an acceleration in the VLM development cycle.

Next to analytical models, the possibility of using numerically solved first-principle models as a method to simulate micro-fluid evaporative flow behaviour has been investigated. The possibilities of several methods have been judged on faithful prediction of flow behaviour, as well as computational stability and costs, which is a large factor in the model's suitability for numerical optimisation.

Of the two investigated first-principle methods, the phase-field method was deemed too computationally expensive to be applied in numerical optimisation, as well as depending heavily on tuned parameters for the functioning of the underlying differential equations. While lower-pressure cases of the applied phase-field method agreed with analytical model predictions concerning complete evaporation, the higher-pressure cases did not agree with the correlated analytical models, with the phase-field simulations requiring double the wall superheat to evaporate the fluid flow (≈ 71 vs ≈ 30 [K]).

In the search for first-principle approaches suitable for numerical optimisation, the Reynolds equation-based two-phase flow method was pioneered, using a set of reduced fluid and heat transfer equations including a smoothly changing phase based on the temperature field. Despite showing promise in speed of simulation for simple cases, this method shows instabilities when applied to more realistic evaporation tests. Extending this approach using a novel 2D form of the Navier-Stokes equation, including the pressure drop calculated using elements of the Reynolds equation, yielded considerable stability improvements compared to the Reynolds equation approach. This novel method is able to very quickly generate simulation results for the investigated abstract two-phase models. This speed-up of computation is expected to provide future venues for two-phase flow numerical optimisation approaches.
5.1.2. DESIGN

Using the analytical model results, the questions concerning the operating parameters posed in chapter 1 (efficiencies, power distribution, minimal wall temperatures) have been answered in chapter 3. Based on these results, and the analysis of operating conditions, several clear design-suggestions are presented.

- The heat transfer will predominantly be from heating-wire to the surrounding silicon base structure, and from the base structure to the fluid. The increase in efficiency due to the use of suspending the heating wires is negligible.

- Due to the explosive behaviour of micro-flow-boiling, the heating wires are liable to be stressed well in excess of acceptable levels. This renders them a likely failure point, and they are as such recommended for redesign. Instead, placement of the resistive heaters on the silicon base structure is suggested as a better alternative, improving both the reliability of the heater elements, as well as improving heat conduction from heater to the whole silicon structure.

- Proposed glass supports by Tiemen van Wees are expected to be sufficiently isolating.

- The power envelop defined in the mission criteria is consequently sufficient for the full operating range.

- Given the current system length for heater and inlet channel, a silicon base temperature of 480[K] is predicted to be sufficient to ensure complete evaporation in all expected operating conditions.

- Pressure drops over the heater are negligible when the rhombi are not included in the final design. When the rhombi are included (as is the case in the current design), the pressure drop remains small, though noticeable in end-of-life operation.

- Transient behaviour will provide little extra requirements, based on the 1D inflow model.

5.2. RECOMMENDATIONS

Next to the conclusions presented above, several items are recommended for further study, both on for future work on modelling two-phase flows, as well as possible design changes.

5.2.1. MODELLING

Though the analytical models have been correlated to available heat-transfer data, validation of the model predictions is to be performed when the TU Delft thrusters are available for testing.

Concerning the phase-field approach: the tunable variables involved in this method greatly influence the phase-field behaviour. Therefore further sensitivity studies on their effect, and concurrent validation experiments on the predicted fluid flow behaviour, are essential before this phase-field technique can be used to predict flows the evaporative micro-fluid flows.

Concerning the applied novel 2D Navier-Stokes equation, extra effort will have to be implemented to improve the stability of the calculations to allow it to be applied to a wider variety of two-phase flows: though simplified fluid-property scenarios are computed fast and without hitch, realistic scenarios show distributed pressure oscillations, which drastically slow down calculations.

5.2.2. DESIGN

Next to the presented design conclusions, this thesis work has unearthed several discussion points concerning the design, where the work so far has not been able to formulate a conclusion:

- As spitting is arguably one of the main propulsion-efficiency impacting factors (save a fully liquid flow-through), preventing this by attempting to have as many as possible fluid-droplet to wall impacts is desirable. This may translates to a staggered column design in the heater chamber, ensuring that no separated liquid droplet can easily float to the nozzle without impacting with some wall along the way. Therefore the limited effect of pillars on the steady-state heat flux minimal temperature requirements, concluded in the presented analytical model, might underestimate the pillar’s effectiveness in preventing liquid flow through the nozzle.
• Concerning spitting, a study of liquid size droplets and the Saffman force might be very useful in understanding this effect, and possibly lead to novel innovations in low-pressure-drop spitting prevention designs.

• Propellant efficiency reported by the analytical study is very high compared to other published experiments with VLM’s. This is due to the much larger expansion ratio designed in the current TU Delft systems. However, the rarefied vapour flow near the end of the nozzle’s expansion will behave differently than the ideal rocket theory calculation predicts, possibly reducing the performance.

• Reverse-flow restrictors in the form of a Tesla-valve or its derived systems might prove valuable in smoothing out the pressure and flow oscillations reported in literature and expected during operation. However in preventing the fluid flow from reversing back into the inlet channel, the resultant effect might conversely increase the risk of liquid being forced into the nozzle.

• Despite the uneven power draw of the fluid (considerably more in the evaporative range), the high thermal conductivity of silicon ensures negligible temperature gradients, allowing for more creative placements of heater elements that might serve ease of assembly, such as external heaters.


This appendix will introduce all needed information on the design of Rob Poyck’s Vaporising Liquid Micro-thruster (VLM). In section A.1 the operation of the full system is explained, while in section A.2 the layout and working principle of the heater element of the thruster will be explained. In section A.4 the dimensions used in this thesis are explained, while in section A.5 the material properties for the structure are introduced. In section A.6 a brief performance summary by [8] is provided, while section A.7 details whether continuum theory can be used for all sections of the VLM. Finally in section A.8 the mounting of the VLM is described.

A.1. VLM: OPERATION

The thruster system is envisioned in a blow-down operation mode, where the propellant is pressurised before launch, and as the propellant is used, the pressure in the storage tank reduces. An overview of this system is shown in figure A.1.

In the storage tank (1) liquid water is held in a flexible bladder, pressurised externally by an inert gas, which sits between the bladder and the metal exterior. The liquid is denoted as blue, while the gas pressurising the liquid outside of the bladder is shown in red.

Using a valve (2), this liquid is allowed to flow to the heater (3) system, where the liquid will be heated and subsequently evaporated. This process transforms the liquid via a region where both liquid an vapour phases are seen, to a fully evaporated vapour, flowing out of the system via the converging-diverging nozzle. If the chamber pressure is high enough, the pressure forces the vapour accelerate up to the local speed of sound in the throat of the nozzle (narrowest point). In the diverging part of the same nozzle, the thermal energy present in the vapour is subsequently used to further accelerate the fluid flow to speeds beyond the speed of sound.

Figure A.1: An abstract overview of the total thruster system, comprised of the propellant storage tank (1), a valve system (2) and the heater (3).
A.2. VLM: DESIGN

The designs created by Poyck included several variants on the same basic principle introduced as the simplified design in figure A.2. At 1, the liquid fluid enters the silicon from the feed-channel, while at 2 the liquid encounters the widening heater chamber. Section 3 is the main heater element. Sections 4 through 6 comprise the nozzle, with a convergent section, the throat, and finally the divergent section.

Figure A.2: The common denominator in the VLM design by Poyck (image from [8]).

Poyck envisioned a readily adjustable design, for any kind of mission. Therefore, his view was to have short but wide heater sections as seen in figure A.3, which can be sequentially repeated to form a larger heater with more heating power, or reduced in number to form shorter heaters for lower-mass-flow VLM’s. The shown heater section includes a large-pillar design: these pillars serve the dual purpose of supporting the heater wires used to heat the fluid, as well interrupting the flow to increasing the heat transfer speed.

Figure A.3: An image of the large diamond heater section (Image from [8]).

These sections are coupled and combined with inlet and nozzle sections to form one of the designs presented by Poyck [8], shown in figure A.4.

Inflow occurs at the left of the system, forced into the system by the pressure contained in the storage tank. As the fluid passes the centre of the heater, the system is heated by wires suspended on top of the pillars, running the width of the system, comprised of a silicon carbide layer. The total expected power draw of each individual section is designed to be ≈1 [W], so any heater of specified power can be assembled, from 1 to 20 [W], or more.

A similar system (sans heating wires) is inverted and mounted on top of the first system, creating the full height of the heater. The nozzle is however only included in one of the two layers, restricting the mass flow of
A.2. VLM: design

Figure A.4: The abstract design by Poyck [8], of the heater envisioned.

Note that the number of pillars in figure A.4, or the dimensions, are not to scale. The small-diamond pattern expected to offer the best performance would use a mask as shown in figure A.5, with subsequently 50 diamonds per row.

Figure A.5: One of the masks used for fabrication, of the small diamond design by [8]

Furthermore, as is seen in figure A.6, on top of those pillars lie the heater wires. These mentioned silicon-carbide wires are isolated from the underlying silicon via a very thin layer of silicon-dioxide. However, as is visible in figure A.6, this layer is fragile as it is only $0.3 \times 6\,\text{mm}$ thick, and prone to breaking during the production process. For instance in the far left, in the middle layer shown, several diamond-shapes are observed to be broken.

Figure A.6: The diamond-shaped columns, with the conductive silicon-carbide layer on top.

The fragileness of these element is in part due to the over-etching of the supported columns (visible as the
lighter diamonds inside the large heater area), reducing the total supported area.

**A.3. OTHER DESIGNS**

Other VLM designs are showed in figure A.7. The Poyck design is somewhat similar to that of Kundu [15], as seen in figure A.7c. However, save the lack of flow-enhancing systems, the wide heater chamber is also found in designs by [16], and in the initial inflow section of the design by [31] (figure A.7e).

**A.4. VLM DIMENSIONS**

The system envisioned by Rob Poyck to satisfy the mission requirements of the QB50 mission, is a heater system with small but numerous diamond pillars. The system dimensions are listed in the table A.1.
A.5. VLM MATERIAL

The material used for the base structure is silicon. Electrically isolating layers are comprised of silicon-dioxide. Highly conductive wires are made of Silicon-Carbide.

As the bulk material is silicon, the thermal conductivity of this material is by far the most important. [18] list the conductivity at 148 [W m$^{-1}$ K$^{-1}$].

Silicon dioxide is listed with a conductivity of $\approx 1.4$ [W m$^{-1}$ K$^{-1}$], about two orders of magnitude less. On the other hand silicon carbide is cited to have a very high conductivity of 490 [W m$^{-1}$ K$^{-1}$], providing very little resistance to heat conduction.

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Table A.1: Approximate dimensions of the VLM for the QB50 mission, as designed by [8].

<table>
<thead>
<tr>
<th>Size</th>
<th>[µ]m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interior heater length</td>
<td>9000</td>
</tr>
<tr>
<td>Interior heater width</td>
<td>3000</td>
</tr>
<tr>
<td>Interior height</td>
<td>150</td>
</tr>
<tr>
<td>Inlet length</td>
<td>1000</td>
</tr>
<tr>
<td>Inlet width</td>
<td>400</td>
</tr>
<tr>
<td>Inlet height</td>
<td>150</td>
</tr>
<tr>
<td>Exterior length</td>
<td>12000</td>
</tr>
<tr>
<td>Exterior width</td>
<td>5000</td>
</tr>
<tr>
<td>Exterior height</td>
<td>3000</td>
</tr>
<tr>
<td>Nozzle throat width</td>
<td>30</td>
</tr>
<tr>
<td>Nozzle exit width</td>
<td>500</td>
</tr>
<tr>
<td>Heater Hydraulic diameter</td>
<td>285.7</td>
</tr>
<tr>
<td>Inlet Hydraulic diameter</td>
<td>218.2</td>
</tr>
</tbody>
</table>

As reported by both Rob Poyck [8] and Tiemen van Wees (unpublished), the DILES production method used to create the heaters using lithography still requires some improvement, especially the vertical etching steps were at times overdone, resulting for instance in the over-etching of support pillars previously seen in figure A.6. The over-etching may also affect other dimensions.

The pillar dimensions, as observed from a horizontal cross section, are listed in table A.2.

<table>
<thead>
<tr>
<th>Size</th>
<th>[µ]m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small pillar length</td>
<td>160</td>
</tr>
<tr>
<td>Small pillar width</td>
<td>40</td>
</tr>
<tr>
<td>Large pillar length</td>
<td>640</td>
</tr>
<tr>
<td>Large pillar width</td>
<td>160</td>
</tr>
</tbody>
</table>

Table A.2: Approximate dimensions pillars, as designed by [8].

The heating wires used for the both the small and large diamond pillar cases have a uniform thickness of 300[nm]. Lengths and widths are shown in table A.3.

<table>
<thead>
<tr>
<th>Size</th>
<th>[µ]m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Small pillar wire length</td>
<td>40</td>
</tr>
<tr>
<td>Small pillar wire width</td>
<td>9</td>
</tr>
<tr>
<td>Large pillar wire length</td>
<td>90</td>
</tr>
<tr>
<td>Large pillar wire width</td>
<td>38</td>
</tr>
</tbody>
</table>

Table A.3: Approximate dimensions pillars, as designed by [8].

Concerning the nozzle: the exit of the nozzle is 16.67 times wider than the throat, therefore the expansion ratio is 16.67. For the nozzle, half of the full heater height is used, as the nozzle is only produced in half of the heater. This is a measure executed to reduce the mass flow rate.
A.6. **VLM: Performance figures**

Robert Poyck calculated that the to have a thrust range of 0.8 to 1.4 [mN], a mission-specific $\Delta V$ of 21.01 [m/s] whilst using less than 6.8 [W], with a mass flow rate of approximately 1 [mg/s] or less, according to [8]. Pressures in the storage tank are expected to vary between 0.5 and 5.5 [bar] absolute pressure.

A.7. **Continuum theory**

The knudsen number for the lowest-pressure case (0.5 [bar]) is calculated by first calculating the average molecular speed, $\bar{v}$ using equation A.1, and applying that to equation A.3:

$$\bar{v} = \sqrt{\frac{8k_B T}{\pi M}} \quad (A.1)$$

Where $k_B$ is the Boltzmann constant ($1.3806504(24) \cdot 10^{23}$ [J K$^{-1}$]), $M$ the molar mass (18 [kg mol$^{-1}$]) and $N_A$ Avogadro’s number ($6.022140857 \cdot 10^{23}$). This element is used to calculate a mean free path using equation A.2, using a viscosity estimate of $1.62 \cdot 10^{-5}$ for vapour, and a density value of 0.23 [kg m$^{-3}$] at the minimum pressure of 0.5 [bar] and a vapour temperature of 473 [K].

$$\lambda = \frac{\mu}{\rho} \sqrt{\frac{\pi M N_A}{2k_B T}} \quad (A.2)$$

The subsequent Knudsen number is $\approx 0.04$ for the low pressure case inside the heater. According to [58] the drag reduction due to Knudsen numbers of 0.1 is 20%. As such, for the sake of this study the continuum theory is used, while acknowledging that a reduction in drag might be appropriate.

However, the nozzle divergent area is currently only half the height of the system. And due to the divergent section of the nozzle, a large reduction in pressure will occur.

According to the work of [23], the continuum approach for the diverging nozzle section can become problematic due to these very low pressures involved. Indeed, pressures of only $\approx 235$[Pa] remain after expansion in the 0.5[bar] feed pressure cases. The Knudsen number calculated for such pressures using equations A.2 and A.3 is well in excess of 10, therefore the continuum approach is not suitable. A further study of these effects lies however outside the scope of this thesis.

Next, using the expected mass flow rates, equation A.5 can be used to estimate the Reynolds numbers in the flow.

$$D_h = \frac{A_{cs}}{2W + 2H} \quad (A.4)$$

$$Re_D = \frac{\dot{m} D_h}{A_{cs} \mu} \quad (A.5)$$

Given initial estimates of approximately $\dot{m} = 1$[mg/s], $D_h = 0.29$[mm] and $A_{cs} = 4.5 \cdot 10^{-7}$[m$^2$] (without pillars), for liquids using $\mu = 10^{-3}$[Pa·s] an estimated Reynolds number is $\approx 0.63$, while for gasses using $\mu = 1.6 \cdot 10^{-5}$[Pa·s] an estimated Reynolds number is $\approx 32$, both clearly laminar. It is therefore safe to assume that the entire studied process is a laminar flow process. Even in the nozzle throat, the Reynolds equation provides numbers less than 140, indicating laminar flow.
A.8. VLM MOUNTING AND OPERATION

As one of the key elements is a limited power budget, care is placed in ensuring that the VLM system is thermally insulated from the satellite frame. To ensure this, Tiemen van Wees presented a solution with small silicon glass cubes (rib length 0.5[mm]) to be placed between the VLM and the underlying PCB.
Creating phase-transfer models

Two options are highlighted to model two-phase evaporative flows in VLM’s: either through the application of simplified 1D analytical models, with correlation coefficients for the heat transfer, or through the use of fundamental fluid equations such as the Navier-Stokes equations, that require numerical solver programs to find a solution. This method is referred to as 'first-principle'-based modelling.

To improve accuracy of the 1D model, the heat transfer parameters are correlated to published data for vaporising liquid micro-thruster (VLM) systems. Two papers who have produced results with comparable designs are introduced and analysed in section B.1.

To allow for the modelling of the VLM heater system with fundamental equations, the methods available in literature are investigated in section B.2.

B.1. Correlation-based modelling

Given the seeming lack of prior art on fully-evaporative analytical models suitable for the VLM’s low mass flux rates, experimental data to correlate new models to is essential. Unfortunately the VLM’s under development at the TU Delft are not currently available for performance evaluation. Therefore existing publications are investigated for operating conditions (mass flux, pressure and temperature range) and device design layout (relatively wide chambers, silicon structure, hydraulic diameters in the sub 0.5[mm] range) to be able to comply with a simplified model of the current TU Delft design by [11]. This system is simplified in the sense that the heat-transfer enhancing structures are omitted for now, representing what is expected to be the worst-case scenario for heat transfer.

Experimental observations published include [31], and [16]. In both cases a silicon structure is created using MEMS technology. The former article details a multi-channel heater structure, while the latter describes a wide open channel heater structure with various produced nozzle openings. As suggested by [18], macro-scale well-known correlations for single-phase heating are applicable to micro-scale models as well. As such, the only unknown concerning heat transfer is the heat flux coefficient in the two-phase regime. To allow a good correlation for the two-phase heat transfer regime, the following two publications are studied.

CEN

A parallel-channel orientated VLM is investigated by [31]. The base structure is silicon, while the top of the structure is manufactured using Pyrex glass, to enable visualisation of the flow (see figure B.1 for the dimensions). An external heater and copper heat-spreader is attached to the silicon base of the VLM. The system has a uniform depth of 120[µm]. The 9 parallel channels each have a width of 80[µm], and are spaced 50[µm] apart.

Several operation cases are described by [31] of their VLM, with mass flows ranging from $2.33 \times 10^{-6} \text{[kg s}^{-1} \text{]}$ to $8.33 \times 10^{-6} \text{[kg s}^{-1} \text{]}$, resulting in mass fluxes ranging from $9.71 \text{[kg m}^{-2} \text{s}^{-1} \text{]}$ to $34.71 \text{[kg m}^{-2} \text{s}^{-1} \text{]}$ (see equation B.1).
CREATING PHASE-TRANSFER MODELS

\[ G = \frac{m}{A_{cs}} \]  

(B.1)

As the expected mass flux for the Poyck design without heat-flux enhancements is approximately \(2.2 \text{ kg m}^{-2} \text{ s}^{-1}\), the lowest mass flow rate is the case to study, with a focus on the inlet section.

The \(2.33 \text{ mg s}^{-1}\) case shows according to \([31]\) intermittent dry-out in the inlet channel, with fewer droplets reaching the parallel duct section. If they did, most of them were observable near the start of this section. Visual data is available to confirm this description.

\([31]\) report that evaporation was indeed sufficient. This suggests that an average length needed for complete evaporation of less than \(4000 \mu\text{m}\). Calculating the hydraulic diameter, an analytic model can be set up, and the point of evaporation tuned by adjusting the heat-flux coefficient for the mixed regime: \(C_{\text{mix}}\). Given the mass-flux similarity to design by \([8]\), it is expected that this correlation factor can be applied to a similar analytic model describing that design.

CHEN

\([16]\) have published an article focused mainly on visually identifying various flow patterns, and assuming complete evaporation, to predict the flow using a full 3D CFD simulation in the aft section of the heater. The layout of this VLM system is more reminiscent of the system designed in the TU Delft by \([8]\): a thin inlet section continues onto a relatively wide and long heater section, followed by a constriction in the form of the nozzle (see figure B.2). The height of the system is \(0.10\text{mm}\), while the width of the main heating chamber is \(1.00\text{mm}\).

\([16]\) have investigated various nozzle cross-sectional areas, however they have not implemented any flow-disrupting structures like the pillars applied by \([8]\).

Observing the case where a nozzle width of \(200 \mu\text{m}\) is used, instead of the reported \(400 \mu\text{m}\) in figure B.2, several interesting cases are observable, as seen in table B.1.

<table>
<thead>
<tr>
<th>Case no.</th>
<th>(T_{\text{wall}}^\circ\text{C})</th>
<th>(\dot{m}) [mg s(^{-1})]</th>
<th>(G) [kg m(^{-2}) s(^{-1})]</th>
<th>Evaporated?</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>150</td>
<td>2.1</td>
<td>21</td>
<td>No</td>
</tr>
<tr>
<td>2</td>
<td>200</td>
<td>2.1</td>
<td>21</td>
<td>Yes</td>
</tr>
<tr>
<td>3</td>
<td>200</td>
<td>4.2</td>
<td>42</td>
<td>No</td>
</tr>
<tr>
<td>4</td>
<td>250</td>
<td>4.2</td>
<td>42</td>
<td>Yes</td>
</tr>
<tr>
<td>5</td>
<td>250</td>
<td>8.3</td>
<td>83</td>
<td>No</td>
</tr>
<tr>
<td>6</td>
<td>300</td>
<td>8.3</td>
<td>83</td>
<td>Yes</td>
</tr>
</tbody>
</table>

Table B.1: Limit cases for non-evaporation and full evaporation, as reported by \([16]\).
Correlating to the paper published by Chen et al. has the benefit of the availability of visual images recorded of the operation of the VLM. This enables a selection of operating points shown in table B.1. Of note is that Chen suggests that even though no liquid is visible in the high mass flux case (8.3[mg s\(^{-1}\)]), the fact that the flow appears not to be choked suggests that still a fraction of the fluid is as of yet un-evaporated [16]. As Chen et al. do not report pressures, this statement is hard to assess using the IRT calculations (a lower pressure is required to force the mass through the nozzle if very fine liquid droplets are present). It has therefore been elected to use the 2.1[mg s\(^{-1}\)] and 4.2[mg s\(^{-1}\)] cases reported, where having a wall temperature of 200 and 250[\(^{\circ}\)C] respectively seems to enable full evaporation.

As the mass-flux numbers are most similar in the lower-mass-flow cases of inlet pressures of 2.1 and 4.2[bar], those are eligible to be used to evaluate heat-flux-coefficients.

Similar to the evaluation of [31], this table can provide some measures to be able to correlate the heat transfer modelled using equation B.2 in the two-phase regime.

\[ q''_s = h(T_w - T) \]  

(B.2)

### B.2. FIRST-PRINCIPLE MODELLING

The analytical models will be based on a 1D perspective. As the VLM design is at least decidedly 2D, including that second (width) dimension in a study of fluid flow behaviour necessitates a finite-element or finite-volume based modelling approach.

Using the fundamental flow and heat equations, it is possible to set up a finite-volume-modelling (FVM) study of the evaporative phenomenon.

For micro-fluid two-phase systems it is apparent that the location of the interface will be a factor in a faithful simulation. It is therefore important to these simulations to be able to distinguish the border between phases, designated as ‘direct numerical simulation of the interface motion’. If the location of the interface is known, effects such as liquid nozzle flow (spitting) can be predicted, and consequently designs can be adjusted to minimise the odds of spitting occurring for the full operating range.

Interface observation is executed using numerous methods, which according to [52] are divided into two sections:

1. By a mathematical relation that explicitly locates the interface in the domain

2. By a marker function that is present in the whole domain, with distinct values of the marker function indicating the phase (for instance a value of 0 for the first phase, and a value of 1 for the second phase, and intermediate marker function results for the interface region)
According to [52] the first approach logically leads to a two-fluid notation, where each phase has its own set of Navier-Stokes equations (or equivalent fluid motion equations), and the interface is advected with a separate set of equations. Note that if separate ‘bubbles’ or phase regions exist, each will have its own separate set of equations, creating even larger issues when a phase region would break up into separate regions. This method lends itself very well to changing-mesh solution methods, where the mesh is deformed to follow the interface exactly, while the highlighted difficulties in bubbles breaking off make it impractical for churning bubbly flows.

The second method using the marker function allows a single-fluid approach, where a single set of Navier-Stokes equations is used for the computation of the velocity field of the fluid in the whole domain, while the properties of the fluids change over the interface, and interfacial effects are effectuated on the Navier-Stokes equations only in the interface region.

Properties of the fluid are determined by an equation like equation B.3. Here \( \alpha \) represents a phase marker function, shifting from 0 in the liquid phase to 1 in the vapour phase, while \( b \) represents some fluid property, with vapour properties denoted as \( b_V \), and liquid properties as \( b_L \).

\[
b = \alpha b_V + (1 - \alpha) b_L \tag{B.3}
\]

This latter approach still requires the application of a suitable marker function, changing the marker distribution to advect the interface, modelling the interface effects and reconstructing the geometry of the interface to allow those interface effects to act. When the interface is explicitly located, the first three tasks also need to be executed, but the interface geometry is already explicitly known.

**Volume-of-Fluid model**

As the single fluid formulation is practical for fixed grids [52], and one of the goals of this thesis is to study the possibility of numerical optimization of the structure confining two-phase flows, this approach is selected, allowing for relatively simple structural fixed-grid optimisation techniques such as density variations of the surrounding structure. [52] applies an improved Volume-Of-Fluid (VOF) model for the determination of the interface location. This method entails the application of an interface-reconstruction algorithm based on weight-functions for each volume element.

The model developed by [52] refers to the slug-flow regime in axi-symmetric ducts. His work mainly focussed on improving the code present in the ANSYS Fluent computer program, and the adjusted code is benchmarked through several (axi-symmetric) cases.

**COMSOL approach**

A very extensive multi-physics computational tool, with built-in finite-volume modelling and solving abilities, is COMSOL MultiPhysics [55]. To solve two-phase flows, they suggest a modelling approach based on a phase-field-based marker function, by Sun and Beckermann [26]. Their model uses the Cahn-Hilliard fourth-order differential equation to advect the phase-field, and implicitly apply the surface tension effects through a body force [59].

The Cahn-Hilliard equation:

\[
\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \nabla \cdot \left( \frac{\omega}{\zeta^2} \nabla \Psi \right) \tag{B.4}
\]

The chemical potential \( \Psi \) is defined as:

\[
\Psi = \omega - \nabla^2 \cdot \frac{\zeta^2}{\kappa} \nabla \phi + \phi (\phi^2 - 1) \phi \tag{B.5}
\]

Here \( \mathbf{u} \) represents the fluid velocity field as usual, while \( \omega [\text{N}] \) represents the mixing density, a function of surface tension \( \sigma [\text{Nm}^{-1}] \) and interface thickness \( \zeta [\text{m}] \), related via B.6:

\[
\sigma = \frac{2^{3/2}}{3} \frac{\omega}{\zeta} \tag{B.6}
\]
Meanwhile, the term $\chi$ denotes the mobility, in $[\text{m}^3 \text{s} \text{kg}^{-1}]$. This term determines the time-scale of the diffusion in the Cahn-Hilliard equation. If this term is increased, the thickness of the interface is restricted, but overly large values dampen the interface motion.

To allow for evaporation, the Cahn-Hilliard equation is modified by adding a term that defines the movement of the phase field based on mass flux from the first phase to the second:

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi - \mathbf{G}_{\text{evap}} \delta \left( \frac{\nu_v}{\rho_v} + \frac{1 - \nu_v}{\rho_L} \right) = \nabla \cdot \chi \omega \zeta^2 \nabla \Psi \tag{B.7}$$

Note that here $\nu_v$ and $\nu_L [\text{m}^3]$ represent the vapour and liquid volume fractions respectively, and $\dot{m}_{\text{evap}} [\text{kg m}^{-2} \text{s}^{-1}]$ represents the mass flux of evaporation. The region where this phase-change occurs is defined by the $\delta$-function, previously seen in equation B.7:

$$\delta = 6\nu_v (1 - \nu_v) \frac{|\nabla \phi|}{2} \tag{B.8}$$

If the investigated fluid domain is envisioned as a 1D system, equation B.8 can be interpreted as a parabolic height-function that centres the acting forces and mass flux at the interface, as in that region it will rise from a zero height value, which ensures that the interface effects can only occur in a region where the gradient of the phase variable is non-zero. This is graphically shown in figure B.3.

Meanwhile, the integration over the full width of the interface resolves in a value of unity, meaning that the integration of the distributed interface effects do amount to the same action that would occur on a mathematically determined thin interface location, as computed using the explicit formulation.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure_B.3.png}
\caption{1D example of the interface $\delta$-function}
\end{figure}

**Evaporation mass flux**

The determination of the mass flux of evaporation is a complicated matter, and as it is of importance on both the approach suggested by Magnini and the approach suggested by COMSOL, it will be expanded upon further.

The production of heat energy due to shear is neglected. Similarly, the radiative heat transmission will also be neglected, as it is expected to constitute only a very small portion of the total heat transfer. This implies that the energy needed to evaporate a fluid will have to be transported to the interface boundary between two phases through conduction.

To better understand this idea, imagine a fluid in a 3D design domain, without gravitational forces, comprised of mainly a liquid with a single evaporated bubble floating in there, while a heater is present some place in
the domain, but not adjacent to the vapour bubble. The vapour bubble must be at least at saturation (boiling) temperature: if it would have a temperature lower than this, gas would condensate against the liquid interface. Let’s assume for now that the vapour is exactly at saturation temperature. If the liquid is to evaporate, a group of molecules in the liquid phase must free itself from the confines of the neighbouring molecules. It can only do so at a vapour-liquid interface with relatively modest extra energy levels, or it must accumulate sufficient thermal energy locally, to allow a vapour bubble to nucleate spontaneously. The latter process is called homogeneous nucleation [60].

For liquid water at atmospheric pressures this temperature is a superheat of about 200[K] (ergo, a total absolute temperature of 573 [K]). This homogenous limit is only reached during very fast heating processes, as normally impurities in the liquid (such as dissolved gasses), or surface roughness cavities holding some trace vapour, allow for a local evaporation process with the interface residing in those places.

In this study homogeneous nucleation will not be further discussed. However, going back to the example, the liquid must be at a higher temperature than the vapour, in order for heat to be transported to the vapour, based on the laws of thermodynamics: heat energy can only flow from the hot source to the cold source. Consequently, the liquid must be at a temperature above the saturation temperature, it must be superheated.

The level of superheat temperature, and through the heat-conduction equation the temperature gradient, will dictate the amount of power transported to the interface. This forms the basis of equation B.9

\[ G_{evap} = -\left(\frac{1}{e_{LH}}\right) n \cdot \kappa \nabla T \]  

\( e_{LH} \) denotes enthalpy of evaporation, \( \kappa \) the local conductivity, \( n \) the unit normal of the interface and \( \nabla T \) the local spatial temperature gradient. This approach mimics the solution proposed by [61], which according to [52] is accurate enough for many macroscopic effects, but neglects the possible temperature discontinuity that may arise in microscopic boiling, as the pressure induced by the surface tension may induce a significant saturation temperature difference between phases.

However, this relatively straight-forward approach is further simplified by COMSOL, as usage of differentiated functions complicate the computations: derivatives may change quicker than the local values, possibly leading to instabilities in the simulation. COMSOL suggest a tunable expression for mass flux instead [55]:

\[ G_{evap} = C \rho_L \frac{T - T_{sat}}{T_{sat}} \]  

Here constant \( C \) denotes a speed-factor for the mass evaporation, a tunable parameter. The tuning of this parameter in the FEM package of COMSOL is deemed important, as too high factors (indicating a fast evaporation speed) may lead to instabilities [55].

Coming back to the argument posed by [52], that a system should allow for a temperature jump, [62] argues that without a temperature jump across the interface, no net flux of molecules is possible. As such, various more inclusive models of the evaporation systems are evaluated.

Magnini presents the theory by Schrage [63] that thermodynamic equilibrium is present in each phase. Schrage also suggests that a temperature jump is present over the interface, relating to the difference in pressure due to the surface tension effect on the pressure. The vapour to liquid mass flux is then expressed as in equation B.11:

\[ G_{evap} = \frac{2}{1} \left(\frac{1}{2\pi R_s}\right)^{1/2} \left(\frac{p_V}{\sqrt{T_V}} - \frac{p_L}{\sqrt{T_L}}\right) \]  

Here \( p_V, p_L \) [Pa], \( T_V \) and \( T_L \) are the vapour and liquid pressure and temperature at the interface, respectively. Tanasawa [62] is cited by Magnini to have derived a simplified equation, where the mass flux is linearly dependent on the temperature jump over the interface (equation B.12). This model is only valid in the case that the temperature jump is significantly less then the vapour temperature near the interface (\( T_{if} - T_V < T_V \)).

\[ G_{evap} = \frac{2}{1} \left(\frac{1}{2\pi R_s}\right)^{1/2} \frac{p_V e_{LH}}{T_V^{3/2}} (T_{if} - T_V) \]  

\[ e_{LH} \] is cited by Magnini to have derived a simplified equation, where the mass flux is linearly dependent on the temperature jump over the interface (equation B.12). This model is only valid in the case that the temperature jump is significantly less then the vapour temperature near the interface (\( T_{if} - T_V < T_V \)).
As in equation B.11, in equation B.12 the vapour temperature at the interface is assumed to lie at the saturation pressure, and that pressure is assumed to be the measurable ‘ambient’ pressure \(T_V = T_{\text{sat}}(p_\infty)\). The equation can be rewritten to be a function of only interface temperature (assigned as the liquid temperature \(T_{\text{if}} = T_L\)) and the vapour pressure:

\[
G_{\text{evap}} = 2 \left( \frac{1}{2\pi R_s} \right)^{1/2} \rho V \frac{\varepsilon L_H}{T_{\text{sat}}} \left( T_{\text{if}} - T_{\text{sat}} \right) = \Phi(p_\infty) \left( T_{\text{if}} - T_{\text{sat}}(p_\infty) \right)
\]  

(B.13)

Here in equation B.13 \(\Phi(p_\infty)\) denotes the collection of variables preceding the linear difference between interface temperature and saturation temperature. It is dubbed the ‘kinetic mobility’ by Tanasawa and Magnini. In other words, the interface temperature is dependent on the local liquid pressure (assuming still a local thermal equilibrium temperature) and as a consequence mainly the surface tension, and the ambient pressure, or the vapour pressure.

When comparing the default suggested evaporation constant \((C = 0.03)\) of COMSOL for equation B.10 to the evaporation speed provided by the Tanasawa equation B.13, a large difference is observed: the default evaporation mass flux constant greatly underestimates the evaporation mass flux, when compared to Tanasawa’s equation. This may have been a conscious act by COMSOL, as they claim it improves stability of the simulation [55].

In the plot shown in figure B.4 better correlating values are suggested, of 1.5[m/s] for the 0.5[bar] case, and 11.5[m/s] for the 5.5[bar] case. These are shown to correlate very well with the values suggested using equation B.13. Bar numerical instabilities, these new factors are to be used in phase-field simulations.

![Figure B.4: Evaporative mass flux as a function of local superheat](image)

Concluding it can be stated that, concerning the difference in approach between COMSOL and the final approach selected by [52], they differ only in choice of constant. COMSOL use liquid density, saturation temperature inversely and a constant C, while the approach by Tanasawa adopted by Magnini uses vapour density, latent heat, saturation temperature to the power of \(-3/2\), molecular weight, coefficient of accommodation and the universal gas constant.

Provided that the difference between the power of \(-1\) used by COMSOL and \(-3/2\) by Magnini is limited, the two approaches are very similar, though the COMSOL approach leans more heavily on empirical constants, and Magnini and Tanasawa use a more thermodynamically reasoned approach. Adjusting the constant C in the COMSOL approach will yield comparable results to the Tanasawa equation, and as such is used, provided that it yields a stable simulation.
B.3. APPENDIX SUMMARY

This appendix investigated available options to model the VLM two-phase flow-boiling behaviour. Initially publications by [16, 31] were evaluated and cases that can be used to correlate 1D analytical models were chosen.

Next the first-principle modelling approach was evaluated, using evaporative flow boiling model by [52] and the approach suggested by [55]. The method for the calculation of the rate of evaporation was compared for the two approaches, and the constant governing this for the COMSOL model (equation B.10) was adjusted to meet the more appropriate modelling by [63] and [62] (equation B.13).
This section of work is intended as a reference for those requiring more insight into the calculated fluid behaviour of the VLM by [8], using the analytical 1D steady-state fluid flow model. Information gathered using the analytical model concerning fluid Reynolds numbers and flow velocities is presented.

### C.1. Reynolds Numbers

The type of flow (purely viscous flow, laminar flow with possible inertial effects, turbulent flow) is evaluated using the Reynolds numbers, visible in figure C.1. The Reynolds numbers for the correlated model simulations range from about 2.5 to just over 250 for the 5.5[bar] case. The maximum numbers are attained in the inlet section.

All reported Reynolds numbers throughout the heater are well in the laminar regime, supporting the choice for a constant Nusselt number of 0.6 [18], as well as the pressure drop calculations used. Inertial effects may play a role in the inlet section, as the guideline suggested by [43] uses $1 \times 10^2$ as the lower limit for flows where inertial effects start to play a role. As this is a steady-state equation, they can be disregarded for this analysis.

In figure C.2 the Reynolds numbers calculated for the system with pillars are shown. Due to the partial cross-sectional obstruction formed by the pillars, the Reynolds numbers past the inlet section have increased compared to the results shown in figure C.1.

### C.2. Flow Velocities

The fluid flow velocities are shown in figure C.3. Several interesting aspects are observable. For instance, the velocities of the 2.0[bar] to 5.5[bar] cases all show a sharp peak at a normalised length of 0.1, while the 0.5[bar] cases show a somewhat more smoothed shift for the higher temperatures (580[K] and up). This is due to the mixed density no longer decreasing, as the majority of the liquid has already evaporated by that point in the 0.5[bar] case, whereas in the higher pressure cases the expansion of the fluid continues, as is seen with the increasing velocity slope.

Furthermore, figure C.3d shows a very slow-moving line for the 430[K], 5.5[bar] case. This is due to the lack of significant evaporation in that case: by the end of the heater only 12.4% of the fluid will have evaporated.

Of the cases that are fully evaporated, a near-identical final velocity is attained for each wall temperature, irrespective of inlet pressure. This is a reasonable result, when we study how that velocity is computed. First using equation C.1 the mass flow through the system is calculated, using mass discharge factor $C_d$, the final chamber pressure $p_c$, the nozzle throat area $A_t$, the Vandenkerkhove function $\Gamma$, final chamber temperature $T_c$ and the specific gas constant $R_s$. Please refer to literature such as [21, 22] for the derivation of the provided equations.

$$\dot{m} = C_d \frac{p_c A_t \Gamma}{\sqrt{R_s T_c}} \quad \text{(C.1)}$$


Figure C.1: Reynolds numbers for varying inlet pressures and wall temperatures

For the fully evaporated fluid (the vapour) the density is approximated for the purpose of this derivation using equation C.2, with $\rho$ the local pressure and $T$ the local temperature.

$$\rho = \frac{p}{R_s T} \quad (C.2)$$

The velocity through the system is computed using equation C.3, based on the mass flow rate, the local density, and the cross-sectional area $A_{cs}$:

$$u = \frac{\dot{m}}{\rho A_{cs}} \quad (C.3)$$

Using now equations C.1 and equation C.2 in equation C.3, the following expression for speed for the fully evaporated liquid can be proposed, as a function the variables for of chamber temperature $T_c$ and local temperature $T$, and chamber pressure $p_c$ and local pressure $p$, and constants as mentioned before.

$$u = \frac{C_d p_c A_{cs}}{p} \frac{p_c A_{cs}}{\sqrt{T_c}} \frac{T}{R_s} \Gamma \quad (C.4)$$

Equation C.4 can be simplified by rearranging the terms to obtain equation C.5, having the variables of pressure and temperature in the leftmost section of the right side of the equation, followed by the constant factors.

$$u = \frac{p_c}{p} \frac{\sqrt{T_c}}{\sqrt{T}} \frac{R_s C_d A_{cs}}{A_{cs} R_s} \Gamma \quad (C.5)$$
As the limited pressure drop over the heater ensures a nearly equal $p_c$ and $p$, the inlet pressure is no longer a factor determining the average speed. After about half the heater’s length, the fluid temperature has generally attained the final chamber temperature. Therefore the remaining factor $\sqrt{T_c}$ determines the magnitude of the velocity. In the 430[K], 5.5[bar] case full evaporation is never attained, and as a result equation C.5 is unable to predict the velocity.

In table C.1 the residence times of the fluid are shown. Due to the lack of evaporation in the 430[K], 5.5[bar] case, and resultant lower velocities, a much larger residence time is visible in the table. Lower wall temperatures show a markedly larger increase in residence time then higher temperature cases. Looking back to figure C.3 this correlates to the much lower velocities of the fluid for the lower temperatures over a relatively large section of the heater, compounding to a larger final residence time.

<table>
<thead>
<tr>
<th>Wall temp [K]</th>
<th>$p_{in} = 0.5$</th>
<th>$p_{in} = 1.5$</th>
<th>$p_{in} = 2.5$</th>
<th>$p_{in} = 3.5$</th>
<th>$p_{in} = 4.5$</th>
<th>$p_{in} = 5.5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>430</td>
<td>0.0178</td>
<td>0.0267</td>
<td>0.0371</td>
<td>0.0527</td>
<td>0.0831</td>
<td>0.2232</td>
</tr>
<tr>
<td>480</td>
<td>0.0142</td>
<td>0.0187</td>
<td>0.0221</td>
<td>0.0255</td>
<td>0.0288</td>
<td>0.0322</td>
</tr>
<tr>
<td>530</td>
<td>0.0127</td>
<td>0.0154</td>
<td>0.0174</td>
<td>0.0192</td>
<td>0.0208</td>
<td>0.0223</td>
</tr>
<tr>
<td>580</td>
<td>0.0114</td>
<td>0.0134</td>
<td>0.0149</td>
<td>0.0160</td>
<td>0.0171</td>
<td>0.0181</td>
</tr>
<tr>
<td>630</td>
<td>0.0111</td>
<td>0.0120</td>
<td>0.0132</td>
<td>0.0141</td>
<td>0.0149</td>
<td>0.0156</td>
</tr>
<tr>
<td>680</td>
<td>0.0097</td>
<td>0.0113</td>
<td>0.0121</td>
<td>0.0127</td>
<td>0.0134</td>
<td>0.0139</td>
</tr>
</tbody>
</table>

Table C.1: Residence times fluxes [s], as calculated with the correlated 1D model, pressures in [bar]

Observing the progression of residence times in table C.1 with increasing pressures but at a constant wall temperature, the final residence times for the 5.5[bar] inlet pressure case are at times the double of the time needed for the 0.5[bar] cases. Using figure C.3, it is clear that the inlet section is passed at a much faster speed in the low pressure cases. As the density of the vapour increases more than 11-fold due to the pressure
increase, this should not come as a surprise. The high-pressure cases require longer heater sections to evaporate. As such the density over the full heater will be on average also higher than the low pressure cases, due to the liquid portion of the two-phase flow remaining present in longer in the higher-pressure cases. All of this compounds to an increase in residence times for the high-pressure cases.

In the rhombi-including design, fluid speeds seen in figure C.4 are slightly larger than those seen in figure C.3: the reduction in available flow area induces a noticeable speed-up. This induces also a reduction in residence times.

The general conclusion of the velocities seen in both figures C.3 and C.4, and exemplified by the residence times shown in table C.1, is that the fluid resides in the heater for a very short time.

The limited residence times hint at fast responses to control inputs to the valve, improving the usability of the system. For instance, for very precise orbit manoeuvres, very short ‘blips’ of thrust might be required.
C.2. Flow Velocities

Figure C.4: Fluid average velocities, for various inlet pressures and wall temperatures
As water is used as the propellant in the VLM thruster, it is important for the accuracy of the models created to have realistic property values.

To facilitate easy incorporation of these matters, the script XSteam.m is used. It provides easy access to the IAPWS IF-97 water and steam property tables, reported to be accurate over a range of 0 - 1000 [bar], and 273 to 2273 [K], according to the IAPWS IF-97 standard [47]. The current standard revisions and updates can be found on the IAPWS website [48].

The script is available from the math-works website, via http://nl.mathworks.com/matlabcentral/fileexchange/9817-x-steam–thermodynamic-properties-of-water-and-steam [46]

At times it might be desirable to indicate an average property, instead of using the embedded lookup-tables. The use of averaged constant values will be indicated.

**D.1. BALANCE MODEL**

All variables included in the balance model are assessed using the steam tables for the heater itself. For the nozzle, constant properties are used, save for the density. Property constants are viewed in table D.1, while the density is determined with equation D.1, with $R_s$ the specific heat constant at 461.9[J/kg], $p$ the pressure [Pa], and $T$ the temperature [K].

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isobaric specific heat $c_p$</td>
<td>2100[J kg$^{-1}$K$^{-1}$]</td>
</tr>
<tr>
<td>Ideal heat ratio $c_p/c_v$</td>
<td>1.3</td>
</tr>
<tr>
<td>Isovolumetric specific heat $c_v$</td>
<td>1615[J kg$^{-1}$K$^{-1}$]</td>
</tr>
</tbody>
</table>

Table D.1: Gas properties.

$$\rho_V = \frac{p}{R_s T} \quad \text{(D.1)}$$

**D.2. 1D STEADY STATE MODEL**

All variables included in the 1D steady-state model in the heater are assessed using the steam tables, while the nozzle vapour properties are calculated using equation D.1 and table D.1.

A critical note must be placed with the determination of the viscosity: averaging the viscosity as performed for this study is a large undervaluation of the complexity. [24] showed several of the possible flow patterns. Based on the various authors cited, slug-flow or annular flow are likely to occur, but mist flow is not excluded either.
As each of the different flow patterns have different degrees of either liquid or vapour coverage of the walls, the averaged viscosity is deemed unsuitable.

Therefore the application of the volume-fraction averaged viscosity here does no predictions concerning type of flow, but assumes a simple flow format where liquid and vapour phases move at the same velocity (homogeneous velocity model). Furthermore, the volume fraction is used as opposed to the mass fraction, as this is a better representation of the total surface area of the section covered by either fluid (on average).

D.3. 1D TRANSIENT MODEL

Gas properties are computed as with nozzle vapour properties, via table D.1 and equation D.1. Furthermore, vapour viscosity is assessed at wall temperature using the steam tables.

Liquid properties are assessed at inflow temperature of 293 [K]:

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Viscosity [Pa s]</td>
<td>$1 \times 10^{-3}$</td>
</tr>
<tr>
<td>Density [kg m$^{-3}$]</td>
<td>998.2</td>
</tr>
<tr>
<td>Isobaric specific heat</td>
<td>4200 [J kg$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>Latent heat energy</td>
<td>$2.2 \times 10^{6}$ [J kg$^{-1}$]</td>
</tr>
</tbody>
</table>

Table D.2: Liquid properties.

The total specific evaporation energy is calculated as the sum of the latent heat, and the product of the isobaric specific heat with the needed temperature increase, from inflow temperature to saturation temperature (also known as the boiling temperature).

D.4. FIRST-PRINCIPLE MODELS

Both vapour and liquid properties are held constant over the range of the simulations. Exceptions are the saturation temperature, which is calculated as a function of the inflow-pressure using the steam tables, and in the case of the realistic scenario, the vapour density, which is calculated using the ideal gas law (equation D.1).

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapour</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg m$^{-3}$]</td>
<td>$\rho_l = 1$</td>
<td>$\rho_v = \rho_l 10^{-n}$</td>
</tr>
<tr>
<td>Viscosity [Pa s]</td>
<td>$\mu_l = 1$</td>
<td>$\mu_v = \mu_l 10^{-1}$</td>
</tr>
<tr>
<td>Conductivity [W K$^{-1}$ m$^{-1}$]</td>
<td>$\kappa_l = 1$</td>
<td>$\kappa_v = \kappa_l 10^{-1}$</td>
</tr>
<tr>
<td>Specific isobaric heat [J kg$^{-1}$ K$^{-1}$]</td>
<td>$c_{p,l} = 1$</td>
<td>$c_{p,v} = c_{p,l} 10^{-1}$</td>
</tr>
</tbody>
</table>

Table D.3: Normalised liquid and scaled vapour properties, for the abstract simulation scenario. Latent heat energy is set to $10$[Jkg$^{-1}$].

<table>
<thead>
<tr>
<th>Property</th>
<th>Liquid</th>
<th>Vapour</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density [kg m$^{-3}$]</td>
<td>$\rho_l = 10^3$</td>
<td>$\rho_v = \frac{\rho_l}{10^7}$</td>
</tr>
<tr>
<td>Viscosity [Pa s]</td>
<td>$\mu_l = 1 \times 10^{-3}$</td>
<td>$\mu_v = 2 \cdot 10^{-3}$</td>
</tr>
<tr>
<td>Conductivity [W K$^{-1}$ m$^{-1}$]</td>
<td>$\kappa_l = 0.6$</td>
<td>$\kappa_v = 0.03$</td>
</tr>
<tr>
<td>Specific isobaric heat [J kg$^{-1}$ K$^{-1}$]</td>
<td>$c_{p,l} = 4.2 \cdot 10^4$</td>
<td>$c_{p,v} = 2 \cdot 10^4$</td>
</tr>
</tbody>
</table>

Table D.4: Realistic liquid and vapour properties. Latent heat is set up as $2.2 \cdot 10^6$[J kg$^{-1}$].

Next to the mentioned properties, the surface tension is held constant at 0.0588[N m$^{-1}$].
REDUCING THE 3D NAVIER-STOKES EQUATION

The Navier-stokes analysis of a 3D system provide a complete laminar analysis, but come at a very high computational cost. For a thin film-like system the application of the Reynolds equations represents a great reduction in computation time, assuming that the Reynolds numbers are sufficiently low. This is attained as firstly the number of elements is reduced greatly from a 3D system to a 2D system, while secondly only a single variable (the pressure variable) describes the full fluid flow, while the Navier-Stokes equation in 3D requires with 4 variables (3 speed components, and pressure) to assess the fluid flow. The Navier-Stokes equation (E.1) and Reynolds equation (E.2) are shown below.

$$\frac{\partial (\rho u_3)}{\partial t} + \nabla \cdot (\rho u_3 \otimes u_3 + p I) = \nabla \cdot \mathbf{r} + \rho \mathbf{g}$$  \hspace{1cm} (E.1)

$$\nabla^2 \left[ \frac{\rho H^3}{12\mu} \nabla p \right] = H \frac{\partial \rho}{\partial t}$$  \hspace{1cm} (E.2)

However, as remarked by [43], from Reynolds numbers of $\approx 1 \times 10^2$ the inertia terms that are neglected in the Reynolds equation might start to play a role again. These have been re-introduced prior by among others [43] to create equation E.3.

$$\frac{\partial (\rho u_2)}{\partial t} + \rho (u_2 \nabla_2) u_2 = -\nabla_2 p + \frac{\mu}{12} u_2 \frac{H^2}{\mu}$$  \hspace{1cm} (E.3)

Like the Navier-Stokes equation, equation E.3 includes the effect of inertia forces, which might become significant for instance in journal bearings [43]. However, unlike the three-dimensional equation E.1, equation E.3 is a 2D equation, simplifying the required modelling. In this latter equation, a total of 3 variables are included: a pressure variable $p$, and a velocity vector $u_2$ with two speed components.

A marked difference between a thin-film-like VLM structure and journal bearings, is the inclusion of flow-interrupting structures like pillars in the former system. To account for such structures, in-plane viscous friction computations need to be enabled. This allows the well known zero-slip boundary condition for walls that restrict the fluid flow domain, as well as internal fluid friction due to velocity differences in-plane.

The resultant equation is similar to a 2D version the Navier-Stokes momentum equation (see equation E.4).

$$\frac{\partial (\rho u_2)}{\partial t} + \rho (u_2 \nabla_2) u_2 = \mu (\nabla^2 u_2 ) - \nabla_2 p$$  \hspace{1cm} (E.4)

It is however augmented with the pressure gradient term $\nabla_2 p = -u_2 \frac{12H^2}{\mu}$, retrieved from the Reynolds Equation, and shown as equation E.5.
\[
\frac{\partial (\rho u_2)}{\partial t} + \rho (u_2 \nabla_2) u_2 = \mu (\nabla_2^2 u_2) - \nabla_2 p + u_2 \frac{12 H^2}{\mu} 
\]  
(E.5)

The assumption of note here is that despite inertia effects becoming a factor, the velocity profile adheres to a parabolic velocity profile. This allows the inclusion of the effects of viscous friction with top and bottom walls in a relatively simple manner.

**E.1. LIMITATIONS TO THE 2D REDUCTION**

When inertial effects start to play a role, a 3D computation of an example system may shows that near obstructions located vertically in the flow system, the parabolic velocity profile is no longer valid and different flow profiles can occur. This could possibly invalidate the assumptions included in equation E.5.

To assess this, a test set-up is created. The fluid domain is shown as the grey solid in figure E.1, while the blue-highlighted pane represents the inlet pane. The outlet pane is not shown.

![Geometry of the test set-up. The solid shown represents the fluid domain.](image)

Figure E.1: Geometry of the test set-up. The solid shown represents the fluid domain.

Table E.1 shows the test parameters used to perform the computation in COMSOL [55]. The pillar who's radius is indicated in the table is placed in the middle of the flow path, as shown in figure E.1. Inflow velocities are dictated over a range from \(1 \times 10^{-3}\) ms\(^{-1}\) to 1 ms\(^{-1}\). The outlet pressure is constrained to a 0 pressure.

<table>
<thead>
<tr>
<th>Dimension</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length</td>
<td>2 mm</td>
</tr>
<tr>
<td>Width</td>
<td>1 mm</td>
</tr>
<tr>
<td>Height</td>
<td>0.15 mm</td>
</tr>
<tr>
<td>Radius pillar</td>
<td>0.25 mm</td>
</tr>
<tr>
<td>Density</td>
<td>(1 \times 10^3) kg m(^{-3})</td>
</tr>
<tr>
<td>Viscosity</td>
<td>(1 \times 10^{-3}) Pas</td>
</tr>
</tbody>
</table>

Table E.1: Comparison test parameters

In figure E.2, one of the outcomes of this test scenario is used as an example: figure E.2a shows the x-component oriented velocity magnitude, as long as it is larger than zero, and aligned with the direction of the x-coordinate vector.

The evolution from the near-uniform velocity field, with little impact from the side-walls, is shown in the first two cross-section panes. The effect of the pillar becomes pronounced already in the 4th cross-section pane, while on from the sixth pane a high fluid velocity remains contained to a relatively small area, smaller at least than would be expected if no inertia effects are included.

Figure E.2b shows where across the shown panes the fluid flows in negative direction, or in reverse direction compared to the orientation of the x-vector. Looking at the cross-section panes after the pillar, it is apparent that a reverse flow occurs in the wake of the pillar.

Perhaps the reader already noted the small discontinuity in the width of the cross-section number 4 in figure E.2a, but in figure E.2b it becomes apparent that a parabolic velocity profile is truly not correct here.
E.2. Qualitative and Quantitative Comparison

To evaluate whether this invalidation of the parabolic flow profile assumption has a major effect, this section will detail the simulation results of a full 3D Navier-Stokes calculation, 2D Navier-Stokes calculations where the third dimension is simply neglected, a Reynolds-equation calculation, and finally the combined equation E.5. The results will be compared on two aspects:

1. Pressure drop over the simulated segment
2. Flow patterns
3. Computation time

The first item is a quantitative measure for the predictability of the simplification proposed, when compared to the full (and costly) 3D computations. The second item represents the question whether the predicted flow patterns by the various methods are alike. If for instance next to the fluid flow a heat transfer system is computed, advection dictated by the fluid flow patterns becomes an important parameter, and accurate flow patterns are required. Finally the third item represents the measure of computation cost required for each scenario, and represents the positive side of the trade-off when decreasing the simulated space from 3D to 2D.

Meshes used for the computations are, for the 3D case, a mesh consisting of $6 \times 10^4$ elements to do a rough initial estimate calculation, and a mesh of $3 \times 10^6$ elements to perform the final calculation. The 2D cases used a mesh of $1 \times 10^4$ elements, with the exception of the final case, where a mesh of $2.7 \times 10^4$ elements was found to provide a much better agreement to the pressure drops reported by the 3D case.

Table E.2 shows the Reynolds-number ranges covered by the computation. The Reynolds numbers are computed using the average velocity over the cross-section:

$$Re = \frac{u \rho D_h}{\mu}$$  \hspace{1cm} (E.6)

Here, $u$ represents the cross-section-averaged velocity, and $D_h$ the hydraulic diameter, calculated as:

$$D_h = \frac{4 A_{cs}}{\phi}$$  \hspace{1cm} (E.7)

Here $A_{cs}$ represents the cross-sectional area, and $\phi$ the wetted perimeter.

As is apparent in table E.2, all Reynolds numbers lie comfortably within the laminar flow range. According to [43] inertia effects can be expected for the final column of tests at an inflow velocity of $1 \text{[m s}^{-1}]$.

<table>
<thead>
<tr>
<th>Inflow velocity</th>
<th>$1 \times 10^{-1}$[m s$^{-1}$]</th>
<th>$1 \times 10^{-2}$[m s$^{-1}$]</th>
<th>$1 \times 10^{-3}$[m s$^{-1}$]</th>
<th>$1$[m s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number max.</td>
<td>0.26</td>
<td>2.56</td>
<td>25.6</td>
<td>256</td>
</tr>
<tr>
<td>Reynolds number min.</td>
<td>0.45</td>
<td>4.46</td>
<td>44.6</td>
<td>450</td>
</tr>
</tbody>
</table>

Table E.2: Reynolds numbers of the various tests
PRESSURE DROP OVER THE SIMULATED SEGMENT

Pressure drops calculated by the system are shown in table E.3. Note that the Reynolds equations provides very predictable results of increasing pressure drops in the same ratio to the increased inflow velocity, which is understandable from the relationship shown in equation E.2. The pressure drops by the 2D Navier-Stokes equation consistently underestimate the total pressure loss, but especially so in the lower inflow speed cases, while in the highest-speed case they show even larger pressure drops than the Reynolds equation. Finally, the combined 2D equation shows a remarkably close computation of the expected pressure drops. This then suggests that while the flow-profile in the height-dimension might not be a parabolic function throughout the system, the approximation holds very well for the computed pressure drops.

<table>
<thead>
<tr>
<th>Inflow velocity</th>
<th>$1 \times 10^{-3}$[m s$^{-1}$]</th>
<th>$1 \times 10^{-2}$[m s$^{-1}$]</th>
<th>$1 \times 10^{-1}$[m s$^{-1}$]</th>
<th>1[m s$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D NS</td>
<td>0.72[Pa]</td>
<td>7.23[Pa]</td>
<td>82.3[Pa]</td>
<td>2960[Pa]</td>
</tr>
</tbody>
</table>

Table E.3: Comparison test results

FLOW PATTERNS

This section will detail the comparison of flow patterns between results of the 3D full Navier-Stokes computation of the introduced test set-up, and the 2D approximations, using either solely the Reynolds number, solely the Navier-stokes computation in 2D (ignoring the out-of-plane viscous friction generated by top and bottom walls), or finally the proposed 2D Navier-stokes computation, with the pressure drop correction, as shown in equation E.5.

In figure E.3 the mid-plane cross-sections of full 3D steady-state Navier-Stokes computation are shown, for the varying inflow velocities. The white arrows indicate the direction of the velocities in the plots, when they are shown. Note that they are not to scale at all times, especially in figure E.3d, as the reverse-flow speeds are markedly smaller, and as such the reverse-flow arrows are enlarged for clarification of the flow pattern.

![Figure E.3: Mid-line velocity plots, with the colour diagrams showing the velocity magnitudes along the x-vector, and scales per image are shown on the right (all velocities in [m s$^{-1}$]).](image)

Note that figure E.3 shows that a wake with reverse flow does not start to fully form until a speed of 1[m s$^{-1}$] has been reached. A low-velocity region is present at lower speeds.

Figure E.4 shows the evolution of the 2D Navier-Stokes equation result. Two marked differences with the 3D case are the earlier start of a reverse-flow wake (from the $1 \times 10^{-1}$[m s$^{-1}$] case shown in figure E.4c), and the
seemingly more 'centred' flow profile. As the only pressure drop arises from friction with the boundaries of the domain shown in the figures, the fluid flowing in the middle of the flow in the low-speed cases experiences very little drag, and consequently this results in a very small predicted pressure drop, shown in table E.3.

Finally in figure E.4d it should be noted that the wake shows signs of oscillatory behaviour, or wake-shedding. This behaviour is not observed in the 3D case, most likely due to the damping friction effects of the top and bottom walls.

Figure E.5 shows the velocity field predicted by the Reynolds equation. As this equation is not bounded by a zero-slip condition at walls, they consequently have no effect on the simulation results, and unrealistic velocity distributions are shown.

Finally figure E.6 shows the results obtained using equation E.5. Comparing the flow patterns to those shown in figure E.3, the resemblance between the flow patterns is striking, including the lack of complete reverse flow in figure E.6c, in contrast to the reported reverse flow by the 2D Navier-Stokes equation in figure E.4c.
E. REDUCING THE 3D NAVIER-STOKES EQUATION

The computation times reported by comsol are depicted in table E.4. The reduction in time spent for the 3D case to any 2D case is striking, though the least-computationally intensive operation remains the Reynolds equation. The computation time reduction for equation E.5 compared to the 3D case varies between approximately a 9 to 65 reduction.

<table>
<thead>
<tr>
<th>Inflow velocity</th>
<th>$1 \times 10^{-3}$ [ms$^{-1}$]</th>
<th>$1 \times 10^{-2}$ [ms$^{-1}$]</th>
<th>$1 \times 10^{-1}$ [ms$^{-1}$]</th>
<th>1 [ms$^{-1}$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>3D NS</td>
<td>191[s]</td>
<td>194[s]</td>
<td>218[s]</td>
<td>301[s]</td>
</tr>
<tr>
<td>2D NS</td>
<td>3[s]</td>
<td>6[s]</td>
<td>28[s]</td>
<td>92[s]</td>
</tr>
<tr>
<td>Reynolds Equation</td>
<td>1[s]</td>
<td>1[s]</td>
<td>1[s]</td>
<td>1[s]</td>
</tr>
<tr>
<td>equation E.5</td>
<td>3[s]</td>
<td>3[s]</td>
<td>4[s]</td>
<td>34[s]</td>
</tr>
</tbody>
</table>

Table E.4: Comparison test results of required computation time for simulations

E.3. CONCLUSIONS

As shown in this chapter, the proposed equation E.5 allows for a large computation time reduction, while limiting the loss in simulation fidelity when compared to the Reynolds equation or simple 2D Navier-Stokes approaches. Based on the tested speed range
Contribution written by Caspar Antonius Jacobus Hanselaar, intended to be submitted with other contributions as a conference paper for the Space Propulsion 2016 conference. (correspondence: caspar.hanselaar@me.com)

F.1. **Abstract (Relevant Addition)**

Performance modelling is presented using analytical methods for boiling flow. This analysis uses a steady-state 1D flow approximation, correlated to published VLM performance data. The applied nozzle flow calculations are adjusted for slit-nozzles, providing a useful tool to quickly predict VLM performance.

F.2. **Method**

Numerical first-principle approaches are rejected as viable simulation methods for this study, as the two-phase evaporative micro-flow simulations currently available are judged not to provide the necessary accuracy and reliability to justify the increased effort in tuning and validation, as well as the increased computation time compared to analytical models.

The performance analysis therefore uses an analytical steady-state modelling approach. Fluid properties are assumed to be continuous functions of enthalpy and pressure. Mass flow rates are determined using the ideal rocket theory, with a nozzle discharge factor of 0.7.

\[
\dot{m} = C_d \frac{p_c A_1 \Gamma}{\sqrt{R_1 T_c}}
\]

The heater is divided in \( n \) shorter sections of length \( \Delta x \). Heat is added to the fluid flow, proportional to the convective heat coefficient and the difference between wall and fluid temperature.

\[
Q = C_{tp} h_{conv} (T_w - T) \Delta x \]

In the two-phase region the heat-transfer coefficients have been correlated to visual references published by [16, 31]. This is implemented using the term \( C_{tp} \). The convection coefficient is determined using equation E3, with the Nusselt number \( Nu \) based on tabulated data for laminar flows.

\[
h_{conv} = Nu \frac{\kappa}{D_h}
\]
The total energy influx can be calculated via equations (F2), the residence time and section length $\Delta x$, to evaluate the enthalpy in the next section.

The pressure drop is calculated using the Kozeny-Carman relation, with $\Phi$, the sphericity of the pillars in the flow, $D_p$, the pillar hydraulic diameter, $\epsilon$ the ratio of volume left after pillars are placed over total volume without pillars, and $u_s$ the superficial velocity calculated without pillars:

$$\frac{\Delta p}{\Delta x} = \frac{180 \mu}{\Phi^2 D_p^2} \left(1 - \epsilon\right)^2 \epsilon^3 u_s$$  \hspace{1cm} (F4)

Consequently using a sufficiently high number $n$ of sections, the average distribution of pressure and enthalpy throughout the fluid flow can be calculated.

Using this data, an insight into the minimal wall temperature needed for full evaporation can be calculated for a given system length. Similarly the pressure drop and mass flow rate can be accurately predicted, providing a more reliable estimate of system performance.

Extending the projections of the system performance to include the thrust levels [mN], the isentropic exit-plane velocities and pressures are determined using the ideal rocket theory [21], knowing the exit-to-throat area ratio. In the computation of the final velocity, an efficiency factor of 0.85 based on the work of [15] has been included to account for the significant boundary layer thickness in the nozzle:

$$F = 0.85 \cdot \dot{m} \cdot u_e + p_e A_e$$  \hspace{1cm} (F5)

The specific impulse values [s] are predicted using the following equation:

$$I_{sp} = \frac{F}{g_0 \dot{m}}$$  \hspace{1cm} (F6)

### E.3. Results

Results of the analytical model are shown below. The plot of figure (F1a) shows the progression of temperature through the heater for an inflow pressure of 2 [bar], and consequently a mass flow varying between 0.37 ($T_w=680$K) and 0.47 [mgs$^{-1}$] ($T_w=430$K). The wall temperature appears to be sufficient to ensure evaporation in all investigated cases. However in the figure (F1b) the inlet pressure of 5.0 [bar] and mass flow rates between 0.93 ($T_w=680$K) and 1.18 [mgs$^{-1}$] ($T_w=430$K) show that the saturation temperature (424.8[K]) is too close to the wall temperature to facilitate sufficient evaporation at low wall temperatures of 430[K].

In figure (F2) the pressure drop registered over the length of the heaters is shown. Despite the flow-interrupting pillars, the pressure drop remains limited to approximately 2.5% in the 2.0[bar] case, and less than 1% in the 5.0[bar] case.

![Figure F.1: Temperatures of the fluid over the normalised length of the heater](image-url)
The thrust levels attained depend mainly on inlet pressure, and to a much smaller extent on the temperature, due to the variance of pressure drop with temperature as seen in figure F.2.

<table>
<thead>
<tr>
<th>Inlet pressure $p_{in}$ [bar]</th>
<th>$F$ [mN] (eq. F.5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>0.23</td>
</tr>
<tr>
<td>2.0</td>
<td>0.47</td>
</tr>
<tr>
<td>3.0</td>
<td>0.71</td>
</tr>
<tr>
<td>4.0</td>
<td>0.95</td>
</tr>
<tr>
<td>5.0</td>
<td>1.19</td>
</tr>
</tbody>
</table>

Table F.1: Thrust values predicted.

Thanks to the minimal pressure drop over the heater, the specific impulse is unaffected by the inlet pressure, and only affected by the wall temperature, as seen in table F.2.

<table>
<thead>
<tr>
<th>Wall temp $T_{we}$ [K]</th>
<th>$I_{sp}$ [s] (eq. F.6)</th>
</tr>
</thead>
<tbody>
<tr>
<td>430</td>
<td>103</td>
</tr>
<tr>
<td>480</td>
<td>109</td>
</tr>
<tr>
<td>530</td>
<td>115</td>
</tr>
<tr>
<td>580</td>
<td>120</td>
</tr>
<tr>
<td>630</td>
<td>125</td>
</tr>
<tr>
<td>680</td>
<td>130</td>
</tr>
</tbody>
</table>

Table F.2: Specific impulse values predicted.

**F.4. CONCLUSION OF CONTRIBUTION**

The proposed correlated analytical steady-state model allows a designer to quickly and accurately investigate minimal wall temperature requirements for a given design proposal. This allows a much faster re-design process than the design-production-test-redesign currently seen in VLM development.

**F.5. DISCUSSION OF CONTRIBUTION**

Current numerical first-principle based methods known to the authors require fine-tuning of parameters to provide realistic results, and come at a significant computational cost. However advancements in this field of simulation will enable the future VLM designer to gain extra insight into the evaporative two-phase flow behaviour, and how different heater-designs can influence this. The combination of accurate numerical fluid-flow results, combined with advancements on numerical topology optimisation, are expected to allow investigations in novel ways on VLM structures.
## F.6. Glossary

<table>
<thead>
<tr>
<th>Variable</th>
<th>Symbol</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density of fluid</td>
<td>$\rho$</td>
<td>[kg m$^{-3}$]</td>
</tr>
<tr>
<td>Viscosity of fluid</td>
<td>$\mu$</td>
<td>[Pa s]</td>
</tr>
<tr>
<td>Conductivity fluid</td>
<td>$\kappa$</td>
<td>[W m$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>Specific gas constant</td>
<td>$R_s$</td>
<td>[J kg$^{-1}$ K$^{-1}$]</td>
</tr>
<tr>
<td>Vandenkerckhove function</td>
<td>$\Gamma$</td>
<td>[1]</td>
</tr>
<tr>
<td>Mass flow</td>
<td>$\dot{m}$</td>
<td>[kg s$^{-1}$]</td>
</tr>
<tr>
<td>Discharge factor</td>
<td>$C_{d}$</td>
<td>[1]</td>
</tr>
<tr>
<td>Nozzle throat area</td>
<td>$A_t$</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>Chamber pressure</td>
<td>$p_c$</td>
<td>[Pa]</td>
</tr>
<tr>
<td>Exit plane pressure</td>
<td>$p_e$</td>
<td>[Pa]</td>
</tr>
<tr>
<td>Chamber temperature</td>
<td>$T_c$</td>
<td>[K]</td>
</tr>
<tr>
<td>Wall temperature</td>
<td>$T_w$</td>
<td>[K]</td>
</tr>
<tr>
<td>Local fluid temperature</td>
<td>$T$</td>
<td>[K]</td>
</tr>
<tr>
<td>Heat transfer correlation coefficient</td>
<td>$C_{tp}$</td>
<td>[1]</td>
</tr>
<tr>
<td>Convective heat transfer coefficient</td>
<td>$h_{conv}$</td>
<td>[J m$^{-2}$ K$^{-1}$]</td>
</tr>
<tr>
<td>Nusselt number</td>
<td>$Nu$</td>
<td>[1]</td>
</tr>
<tr>
<td>Cross-sectional area</td>
<td>$A_{cs}$</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>Wetted perimeter</td>
<td>$\mathcal{P}$</td>
<td>[m]</td>
</tr>
<tr>
<td>Hydraulic diameter heater cross-section</td>
<td>$D_h$</td>
<td>[m]</td>
</tr>
<tr>
<td>Hydraulic diameter pillar</td>
<td>$D_p$</td>
<td>[m]</td>
</tr>
<tr>
<td>Sphericity pillars</td>
<td>$\Phi_s$</td>
<td>[1]</td>
</tr>
<tr>
<td>Volume fraction remaining with pillars</td>
<td>$\epsilon$</td>
<td>[1]</td>
</tr>
<tr>
<td>Section length</td>
<td>$\Delta x$</td>
<td>[m]</td>
</tr>
<tr>
<td>Superficial velocity</td>
<td>$u_s$</td>
<td>[m s$^{-1}$]</td>
</tr>
<tr>
<td>Exit plane velocity</td>
<td>$u_e$</td>
<td>[m s$^{-1}$]</td>
</tr>
<tr>
<td>Exit plane area</td>
<td>$A_e$</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>Residence time</td>
<td>$\tau$</td>
<td>[s]</td>
</tr>
<tr>
<td>Thrust force</td>
<td>$F$</td>
<td>[N]</td>
</tr>
<tr>
<td>Specific impulse</td>
<td>$I_{sp}$</td>
<td>[s]</td>
</tr>
<tr>
<td>Gravitational acceleration</td>
<td>$g_0$</td>
<td>[m s$^{-2}$]</td>
</tr>
</tbody>
</table>

Table F.3: Glossary of symbols used
ABSTRACT PROPOSAL: ANALYTICAL AND FIRST-PRINCIPLE BASED EVAPORATIVE FLOW MODELLING FOR VAPORIZING LIQUID MICRO-THRUSTERS

For cubesats the race for an adequate yet simple propulsion method is on. Vaporizing liquid micro-thrusters appear to be one of the viable solutions to provide this. However, little to no two-phase fluid-flow modelling has been performed so far in the design of VLM systems.

Two-phase evaporating models published so far focus on high mass-flux (> 100 [kg m$^{-2}$ s$^{-1}$]) cooling of integrated circuits, and on low vapour fraction operation. By contrast, VLM systems require all of the fluid to be evaporated for optimal performance. To ensure this, low mass-flux (< 30 [kg m$^{-2}$ s$^{-1}$]) systems are generally used.

This mismatch ensures that evaporation models cannot be freely exchanged. This paper therefore presents two methods of investigating two-phase fluid flow behaviour in VLMs: an analytical, and a first-principle approach. The analytical approach is correlated using visual data available in published literature. The first-principle approach uses a novel adaptation of the Reynolds equation, with a reintroduction of both inertia terms and viscous friction terms of in-plane fluid motion.

The first method is shown to provide clear and fast insights in VLM operation, and is a valuable tool in the design methodology, allowing for the identification of minimal wall temperatures, efficiency values and performance values. Despite the presence of numerical oscillations, the first-principle approach shows promise, as it reduces the computation time of two-phase fluid flow systems drastically compared to the phase-field method used as the reference.

Keywords:
Vaporizing Liquid Micro-thruster, Micro-fluidics, MEMS, Navier-Stokes equations, Reynolds Equation, Two-phase flow
Three types of analytical model are used:

1. Balance model
2. Steady-state 1D model
3. Transient 1D model

This section will provide the MatLab script code used to perform the calculations.

H.1. Balance model

%% BalanceModels.m %%
% This file is intended to quickly assess system parameters when designing
% a VLM thruster. Accounted for is:
% 1. Heating power required to attain desired temperature for prescribed
%    inlet pressure and nozzle dimensions
% 2. Expected radiative power loss, based on an aluminized exterior
%    emittance of 0.05 [Mills1999, table A.5a]
% 3. Expected conductive power loss based on glass support structures
%    with a thermal conductivity of 1.09 [W/(m*K)], based on
%    [Mills1999, table A.3]
%
% File created by C.A.J. Hanselaar, on december 29th, 2015, for the MSc.
% thesis project
% Final cleanup of file occured on March 3rd, 2016, by CAJ Hanselaar

%% Startup:
clear all

%% Input values
T_in_C = 20; % [C] Input temperature
T_in = T_in_C + 273; % [K] Input temperature
T_out_base_C = 157; % [C] Minimum of investigated temperature range

%% Material constants
k_Si = 149; % [W/(m*K)] Conductivity of silicon base structure
k_g = 1.09; % [W/(m*K)] Conductivity of glass support
em = 0.05; % [1] Emittance factor of exterior
Rs = 8314 / 18; % [J/kg/K] Specific gas constant for water
\[ \gamma_{\text{ideal}} = 1.3; \quad \% \text{[1] specific heat ratio} \]
\[ \text{VDK} = 0.6673; \quad \% \text{[1] VanDenKerckhove Function parameter} \]
\[ g_0 = 9.81; \quad \% \text{[m/s}^2\text{]} \text{ Gravity acceleration} \]

%% Internal dimensions of the system
%% Heater chamber
\[ L_{\text{int}} = 10e^{-3}; \quad \% \text{[m] Interior Length of heater} \]
\[ W_{\text{int}} = 3e^{-3}; \quad \% \text{[m] Interior Width of heater} \]
\[ H_{\text{int}} = 0.15e^{-3}; \quad \% \text{[m] Exterior Height of heater} \]

%% Nozzle structure
\[ W_t = 30.1e^{-6}; \quad \% \text{[m] Throat width} \]
\[ A_t = H_{\text{int}}/2 \times W_t; \quad \% \text{[m}^2\text{]} \text{ Throat area} \]
\[ W_e = 500e^{-6}; \quad \% \text{[m] Nozzle exit width} \]
\[ A_e = W_e \times H_{\text{int}}/2; \quad \% \text{[m}^2\text{]} \text{ Nozzle exit area} \]
\[ A_{\text{ratio}} = A_e / A_t; \quad \% \text{[1] Nozzle expansion ratio} \]
\[ C_d = 0.7; \quad \% \text{[1] Mass ejection fraction expectation} \]
% NOTE: ejection fraction based on the work of [Krusharev] and [Kundu]

%% External dimensions of the system
\[ L_{\text{ext}} = 20e^{-3}; \quad \% \text{[m] Exterior Length of heater} \]
\[ W_{\text{ext}} = 10e^{-3}; \quad \% \text{[m] Exterior Width of heater} \]
\[ H_{\text{ext}} = 3e^{-3}; \quad \% \text{[m] Exterior Height of heater} \]
\[ A_{\text{ext}} = L_{\text{ext}} \times W_{\text{ext}} \times 2 + ... \]
\[ H_{\text{ext}} \times L_{\text{ext}} \times 2 + ... \]
\[ H_{\text{ext}} \times W_{\text{ext}} \times 2; \quad \% \text{[m}^{-2}\text{]} \text{ Exterior dimensions of the system} \]

%% Loop for Power requirements
for k1 = 1:6;
for k2 = 1:11;
% Target values
% Adjusted here so a range of operating points is simultaneously
% investigated, and plotted at the end of the file
% Expected vapour output temperature at the end of the heater
\[ T_{\text{out,C}} = T_{\text{out base,C}} + (k1-1) \times 50; \% \text{[C] Input temperature} \]
\[ T_{\text{out save}}(k1,k2) = T_{\text{out,C}}; \]
\[ T_{\text{out}} = T_{\text{out,C}} + 273; \quad \% \text{[K] Output temperature} \]
% Inflow pressure into the heater
\[ P_{\text{in,Bar}} = 0.5 + 0.5 \times (k2-1); \quad \% \text{[Bar] Input pressure} \]
\[ P_{\text{in save}}(k1,k2) = P_{\text{in,Bar}}; \]
\[ P_{\text{in}} = P_{\text{in,Bar}} \times 10^5; \quad \% \text{[Pa] Input pressure} \]

%% Internal heat required
% The required energy is calculated using fluid input and desired fluid
% output temperature, at inflow pressure, as the pressure drop in the
% heater is assumed to be minimal.
% Energy required based on enthalpy
\[ T_{\text{sat,C}} = \text{XSteam('Tsat_p',P_{\text{in,Bar}})}; \quad \% \text{[C] Saturation temperature} \]
\[ T_{\text{sat}} = T_{\text{sat,C}} + 273; \quad \% \text{[K] Saturation temperature} \]
\[ h_{\text{tot,kJ/kg}} = \text{XSteam('h_pT',P_{\text{in,Bar}},T_{\text{out,C}})}; \]
% Mass flow expected
\[ m_{\text{flow}} = C_d \times P_{\text{in}} \times A_t \times VDK; \]
(Rs * T_out)^.5; % [kg/s] Mass flow through nozzle
m_flow_save(k1,k2) = m_flow;

% Computed needed power based on expected mass flow
P_fluid = (h_tot_J_kg) * m_flow;

%% Radiative lossess expected
% Radiation loss calculation, using wall temperature input in Kelvin, and
% radiative surface area in m^-2, the emissivity of the used material [1] and
% the surrounding temperature in [K]
% The output is the projected power loss through radiation.
T_surr = 0; % surrounding temp in K
T_surf = T_out; % surface temperature in K

% Power flow due to radiation, assuming the scenario where the
% entire silicon structure is at the wall temperature.
sigma_stef_bolz = 5.670373*1e-8; % J/(s * m^2 * K^4)
P_rad = (T_surf^4 - T_surr^4)* em * ...
sigma_stef_bolz * A_ext; % J/s

%% Conductive lossess expected
% The conductive lossess are calculated based on several assumptions:
% 1. The support structure is at fluid inflow temperature
% 2. The link between heater and support structure is based on a glass
% frame
% 3. The heater exterior temperature is the same as the heater interior
% wall temperature due to the high thermal conductivity of silicon
T_struct = T_in; % [C] support structure temperature
K_struct = k_g; % [W/(m*K)] approx value glass
L_struct_cond = 0.5e-3; % [m] length of structure
A_cs_struct_cond = (L_struct_cond)^2 *4; % [m^2] cross section of support pillars
P_cond = (T_out-T_struct)*...
A_cs_struct_cond/L_struct_cond*k_struct; % [W] Conduction loss power

%% Total power requirements
P_tot = P_fluid + P_rad + P_cond; % total heating power required
eta_tot = P_fluid / P_tot; % Heating efficiency
P(k1,k2) = P_tot; % Storage of power requirement
P_fl(k1,k2) = P_fluid; % Storage of fluid power requirement
P_c(k1,k2) = P_cond; % Storage of conductive power losses
P_r(k1,k2) = P_rad; % Storage of radiative power losses
eta(k1,k2) = eta_tot; % storage of heating efficiency

%% Thrust expectation
% This section is based on the class notes for thermal rocket propulsion by B. Zandbergen, and Sutton
% Calculation of the pressure, based on a numerical assessment
[Pe,~,~] = PressureEvalFun(P_in,gamma_ideal,A_ratio,VDK);
p_e(k1,k2) = Pe; % storing the pressure
% Calculating the expected final velocity:
u_e = sqrt(2 * (gamma_ideal/(gamma_ideal-1)) * Rs * T_out * ...
(1- (Pe / P_in)^(gamma_ideal-1)/(gamma_ideal-1)/gamma_ideal)); % Calculating the force generated using velocity, expected velocity
% efficiency (based on Kundu and Krusharev), mass flow, pressure
% and exit area
\[ F(k1,k2) = m_{\text{flow}} \cdot u_e \cdot \eta_v + \text{Pe} \cdot A_e; \]
\% Calculating the specific impulse figure
\[ I_{\text{sp}}(k1,k2) = F(k1,k2)/m_{\text{flow}}/g0; \]
end;
end;

**H.2. STEADY-STATE MODEL**

%% SteadyStateModel_1D.m
% This model is based on a steady-state power distribution model for a
% Vaporizing Liquid Microthruster.
% This file corresponds to the VLM by R. Poyck (2014). Note that the
% correlation factor of 2.75 corresponds to the correlation performed with
% data form Cen and Chen.
% Main assumptions
% 1. The fluid only flows in the length-wise direction from inlet to
% outlet, and pressure drop is modeled using Poiseuille flow.
% 2. All fluid properties are uniform in any cross-section perpendicular
% to the flow direction.
% 3. All thermodynamic processes are at steady-state
% 4. Heat transfer is modelled using Nusselt correlations as in Bergman
% and Incropera for pure phase fluids
% 5. Even though the model concerns a very thin fluid, no full occlusion
% by vapour bubbles is assumed. Instead, an ideal mixture is assumed,
% as per large-scale boiling systems. This fails to model some of the
% explosive-boiling phenomena observed in experiments, but
% facilitates computation of a 1D system
% 6. No heat conduction via the liquid along the flow direction is
% accounted for, to simplify the calculations.
% File created by C.A.J. Hanselaar for the MSc. thesis project

%% Startup
clear all
plotting = 1;
C_evap = 2.75;
RhombiBoolean = 1;
% Note that the RhombiBoolean allows for a switch between the case where
% the pressure is studied using the 1D reynolds equation, or the case where
% the Kozeny-Carman relation is used for pressure drop. The former is
% appropriate for an 'empty'-chamber design, while the latter corresponds
% to the flow-interrupting pillar design by Rob Poyck.
% Important parameter for the latter case are the porosity ratio (eps1),
% defined as the volume not occupied by pillars or columns, and the
% sphericity (Sph), assumed as unity for now.

for ct_out = 1:10;
    T_{wall}_start=157+(ct_out-1) * 30;
    T_{fluid}_in = 20;
    p_{start} = 1;
    Cd_{input} = 0.7;
    % System input settings
    % Implemented to allow external execution of this file based on the pre-set
    % wall values T_{wall}_start (C), fluid input value T_{fluid}_in (C) and pressure value
    % p_{start} (bar)
    try
        T_{wall}_C = T_{wall}_start;% [C] Wall temperature
% Steady-State Model

T_in_C = T_fluid_in; % [C] Fluid inlet temperature
p_in_bar = p_start; % [bar] Fluid inlet pressure
Cd = Cd_input; % [1] Ejection fraction nozzle

catch
disp('Sorry Dave, I cannot do that...')
disp('There is no starting temp or pressure defined, please provide input: ')
disp(')
T_wall_C = input('What is the starting wall temperature [C]? ');
T_in_C = input('What is the starting fluid temperature [C]? ');
p_in_bar = input('What is the input fluid pressure [bar]? ');
Cd = input('What is the discharge coefficient for the IRT? ');
disp('...');pause(0.5)
disp('Thank you, Dave...');pause(0.5)
disp('...');
end

T_in_K = T_in_C + 273.15; % [K] Fluid inlet temperature in Kelvin
T_wall_K = T_wall_C + 273.15;% [K] Wall temperature in Kelvin
p_in_Pa = p_in_bar * 1e5; % [Pa] Fluid inlet pressure in Pascal

% Property definitions
% List of pre-determined material properties and other general definitions
% needed for the computation

% Silicon heater properties
k_Si = 149; % [W/(m*K)] Conductivity of silicon base structure
k_g = 1.09; % [W/(m*K)] Conductivity of glass support
em = 0.05; % [1] Emittance factor of exterior

% Fluid properties
Rs = 8314 / 18; % [J/kg/K] Specific gas constant for water
gamma_ideal = 1.3; % [1] Specific heat ratio for vapour, assumed constant
VDK = 0.6673; % [1] VanDenKerkhove Function parameter

% general definitions
g0 = 9.81; % [m/s^2] Gravity acceleration
Nu = 6; % [1] Nusselt number estimate based on Bergman2011
if RhombiBoolean ==1
    C_Wang = 2; % Doubling of nusselt number based on Wang2011
else
    C_Wang = 1;
end;

% System dimensions
% Includes all geometric definitions needed to perform the calculations.
% Note that the geometry used is a simplification, assuming no structures
% obstructing the flow, such as the pillars in the design of Poyck and
% Krusharev.

% Heater chamber
L_int = 1e-3; % [m] Interior Length of heater
L_inlet = 1e-3; % [m] Inlet Length of heater, no heat flux here
W_int = 3e-3; % [m] Interior Width of heater
W_inlet = 0.4e-3; % [m] Interior Width of inlet section
H_int = 0.15e-3; % [m] Interior Height of heater
H_inlet = 0.15e-3; % [m] Interior Height of inlet section
\( A_{cs} = W_{\text{int}} \times H_{\text{int}}; \) \([\text{m}^2]\) Cross section
\( A_{cs,\text{inlet}} = W_{\text{inlet}} \times H_{\text{inlet}}; \) \([\text{m}^2]\) Cross section
\( \text{Perim} = W_{\text{int}} \times 2 + H_{\text{int}} \times 2; \) \([\text{m}]\) Length of perimeter at each cross-section
\( \text{Perim,\text{inlet}} = W_{\text{inlet}} \times 2 + H_{\text{inlet}} \times 2; \) \([\text{m}]\) Length of perimeter at each cross-section
\( \text{Dh} = 4 \times A_{cs} / \text{Perim}; \) \([\text{m}]\) Hydraulic diameter heater
\( \text{Dh,\text{inlet}} = 4 \times A_{cs,\text{inlet}} / \text{Perim,\text{inlet}}; \) \([\text{m}]\) Hydraulic diameter inlet
\( Dp_h = \frac{(4 \times (40e-6 \times H_{\text{int}})))}{(2 \times 40e-6 + 2 \times H_{\text{int}})}; \) \([\text{m}]\) Frontal Dh of pillars
% Note: the hydraulic diameter of the pillars, for the rhombi-p-drop.
\( \text{eps1} = 0.67; \) \([\text{1}]\) Porosity determined by Poyck2014
\( \text{Sph} = 1; \) \([\text{1}]\) Sphericity of pillars, assumed at unity
% Nozzle structure
\( W_t = 30.1e^{-6}; \) \([\text{m}]\) Throat width
\( A_t = H_{\text{int}} / 2 \times W_t; \) \([\text{m}^2]\) Throat area
\( W_e = 500e^{-6}; \) \([\text{m}]\) Nozzle exit width
\( A_e = W_e \times H_{\text{int}} / 2; \) \([\text{m}^2]\) Nozzle exit area, in half the system
\( A_{\text{ratio}} = A_e / A_t; \) \([\text{1}]\) Nozzle expansion ratio
\( \text{eta}_v = 0.85; \) \([\text{1}]\) Expected velocity efficiency nozzle
% Exterior dimensions
\( L_{\text{ext}} = 20e^{-3}; \) \([\text{m}]\) Exterior Length of heater
\( W_{\text{ext}} = 10e^{-3}; \) \([\text{m}]\) Exterior Width of heater
\( H_{\text{ext}} = 3e^{-3}; \) \([\text{m}]\) Exterior Height of heater
\( A_{\text{ext}} = L_{\text{ext}} \times W_{\text{ext}} \times 2 + \ldots + H_{\text{ext}} \times W_{\text{ext}} \times 2; \) \([\text{m}^2]\) Exterior dimensions of the system
%
\% Discretisation
\( n_{\text{it}} = 5000; \) \([\text{1}]\) Number of spatial steps
\( dx = L_{\text{int}} / n_{\text{it}}; \) \([\text{m}]\) Length of spatial step
\( x = [0:dx:n_{\text{it}} \times dx]; \) \([\text{m}]\) Length of heater
\( A_{\text{cond}} = \text{Perim} \times dx; \) \([\text{m}^2]\) Area for internal heat conduction
%
\% Conductive lossess expected
% The conductive lossess are calculated based on several assumptions:
% 1. The support structure is at fluid inflow temperature
% 2. The link between heater and support structure is based on a glass frame
% 3. The heater exterior temperature is the same as the heater interior wall temperature due to the high thermal conductivity of silicon
% 4. Support pillars consist of small 0.5 [mm] glass cubes, isolating the heater from the support, as per suggestion of T. Wees, BSc.
\( T_{\text{struct}} = T_{\text{in,K}}; \) \([\text{C}]\) support structure temperature
\( k_{\text{struct}} = k_g; \) \([\text{W/(m*K)}]\) approx value glass
\( A_{\text{cs,struct,cond}} = (0.5e^{-3})^2 \times 4; \) \([\text{m}^2]\) cross section of support pillars
\( L_{\text{struct,cond}} = 0.5e^{-3}; \) \([\text{m}]\) length of structure
\( P_{\text{cond,struct}} = (T_{\text{wall,K}} - T_{\text{struct}}) \times \ldots \times A_{\text{cs,struct,cond}} / L_{\text{struct,cond}} \times k_{\text{struct}}; \) \([\text{W}]\) Conduction loss power
%
\% Radiative lossess expected
% Radiaton loss calculation, using wall temperature input in Kelvin, and radiative surface area in m\(^2\), the emissivity of the used material [1] and the surrounding temperature in [K]
\( T_{\text{surr}} = 20; \) \([\text{K}]\) surrounding temp in Kelvin
\( T_{\text{surf}} = T_{\text{wall,K}}; \) \([\text{K}]\) surface temperature in Kelvin
% Power flow due to radiation, assuming the scenario where the entire silicon structure is at the interior wall temperature.
\[
\sigma_{\text{stef bolz}} = 5.670373 \times 10^{-8} \text{ [J/(s} \cdot \text{m}^2 \cdot \text{K}^4]\}
\]
\[
P_{\text{rad}} = (T_{\text{surf}}^4 - T_{\text{surr}}^4) \times \text{em} \times ...
\]
sigma_{\text{stef bolz}} \times A_{\text{ext}}\% [W]

%% Loop
% Determining initial mass flow estimate:
\[
m_{\text{flow}} = C_d \times p_{\text{in}} \times A_t \times \text{VDK} / ...
\]
\[
(R_s \times T_{\text{wall}})^{-0.5}; \% [kg/s] Mass flow through nozzle
go=1;
ct2 =1;
while go==1;
% Clearing prior calculation results
clear ent_fl p_fl_bar T_sat_C T_fl_C P_fl
clear x_vap rho kappa_fl v t_total my_fl
% Starting criteria:
t_{\text{total}}(1) = 0; \% starting time is 0 [s]
p_{\text{fl_bar}}(1) = p_{\text{in}}; \% pressure [bar]
T_{\text{fl_C}}(1) = T_{\text{in}}; \% temperature [C]
% Calculating enthalpy using XSteam tables and input pressure and temp
ent_fl(1) = XSteam('h_pT', p_{\text{fl_bar}}(1), T_{\text{fl_C}}(1)); \% kJ/kg
% Starting run
for ct = 1:n_it; \% Simulating steady-state heat transfer and phase change
% Determining properties
% assessing saturation temperature
T_{\text{sat_C}}(ct) = XSteam('Tsat_p', p_{\text{fl_bar}}(ct)); \% saturation temperature [C]
% Calculating fluid temperature
T_{\text{fl_C}}(ct) = XSteam('T_ph', p_{\text{fl_bar}}(ct), ent_fl(1)); \% [C]
% Calculating enthalpy, using input pressure and enthalpy
x_vap(1) = XSteam('x_ph', p_{\text{fl_bar}}(ct), ent_fl(1)); \% [1]
% Calculating average density, using input pressure and enthalpy
rho(1) = XSteam('rho_ph', p_{\text{fl_bar}}(ct), ent_fl(1)); \% [kg/m3]
% Calculating thermal conductivity
kappa_fl(1) = XSteam('tc_ph', p_{\text{fl_bar}}(ct), ent_fl(1)); \% [W/m/C]
\]
% Current state check, using calculated vapour fraction x_vap
if x_vap(1) >= 0.9995
% Gass state
x_vap(1) = 1;
% In the case of a marginally vaporized liquid (0.9995 <x_vap<1),
% to prevent errors, we add a small percentage of heat to the fluid, to set the system to have enough energy to be considered a gas. This prevents errors mainly in the XSteam lookup tables.
if ent_fl(1) < XSteam('hV_T', T_{\text{sat_C}}(ct));
ent_fl(1) = XSteam('hV_T', T_{\text{sat_C}}(ct)+0.01);
end;
% Calculating average viscosity
my_fl(1) = XSteam('my_ph', p_{\text{fl_bar}}(ct), ent_fl(1)); \% [Pa * s]
else if x_vap(1) > 0;
% Mixture state
% Calculating average viscosity
my_fl_L = XSteam('my_pT','p_fl_bar(ct),T_fl_C(ct)-1); % [Pa * s]
my_fl_V = XSteam('my_pT','p_fl_bar(ct),T_fl_C(ct)+1); % [Pa * s]
my_fl(ct) = vx_vap(ct) * my_fl_V + (1-vx_vap(ct)) * my_fl_L;
kappa_fl(ct) = XSteam('tc_pT','p_fl_bar(ct),T_sat_C(ct)+1)*vx_vap(ct) + ...
XSteam('tc_pT','p_fl_bar(ct),T_sat_C(ct)-1)*(1-vx_vap(ct)); % [W/m/C]
else
% Liquid state
% Calculating average viscosity
my_fl(ct) = XSteam('my_ph','p_fl_bar(ct),ent_fl(ct)); % [Pa * s]
end;

%% Pressure and velocity calculations
if x(ct+1) >=L_inlet
if RhombiBoolean ==1
v(ct) = m_flow / (rho(ct)*W_int*H_int * eps1);% [m/s] Average fluid speed, accounting for obstructions by rhombi
vs = m_flow / (rho(ct)*W_int*H_int);% [m/s] Superficial velocity
dt = dx / v(ct); % [s] Time used to cross section of heater
dp_Pa = 180 * my_fl(ct) / (Sph^2*Dp_h^2) * (1-eps1)^2 / eps1^3 * vs * dx;
Re(ct) = m_flow * Dh / (A_cs*eps1) / my_fl(ct);
else
v(ct) = m_flow / (rho(ct)*W_int*H_int);% [m/s] Average fluid speed, no rhombi
dt = dx / v(ct); % [s] Time used to cross section of heater
dp_Pa = 12 * my_fl(ct) * v(ct) / H_int^2*dx; % [Pa]
Re(ct) = m_flow * Dh / (A_cs * my_fl(ct));
end;
else
v(ct) = m_flow / (rho(ct)*W_inlet*H_inlet);% [m/s] Average fluid speed
dt = dx / v(ct); % [s] Time used to cross section of heater
dp_Pa = 12 * my_fl(ct) * v(ct) / (H_inlet)^2*dx; % [Pa]
Re(ct) = m_flow * Dh_inlet / A_cs_inlet / my_fl(ct);
end;

%% Heat flow
if x_vap(ct) < 0.9995
if x_vap(ct) >0
C_h = C_evap;
else
C_h = 1;
end;
else
C_h = 1;
end;
if x(ct+1) >=L_inlet
% assessing whether the inflow length has been superceded
hc(ct) = C_h * C_Wang * Nu * kappa_fl(ct) / Dh; % [W/K/m^2]
q = hc(ct) * (T_wall_C - T_fl_C(ct)); % [W/m^2]
Q = q * Perim * dx; % [W]
E = Q * dt; % [J]
dE_dm = E / (rho(ct) * (A_cs) * dx); % [J/kg]
dE_dm_KJ = dE_dm/1e3; % [kJ/kg]
P_fl(ct) = Q; % [W]
else
hc(ct) = C_h *Nu * kappa_fl(ct) / Dh_inlet; % [W/K/m^2]
q = hc(ct) * (T_wall_C - T_fl_C(ct)); % [W/m^2]
Q = q * Perim_inlet * dx; % [W]
E = Q * dt; % [J]
\[ \text{d}E_{\text{dm}} = \frac{E}{(\rho(\text{ct}) \cdot (A_{\text{cs_inlet}}) \cdot \text{dx})}; \quad [\text{J/kg}] \]
\[ \text{d}E_{\text{dm}} \text{kJ} = \frac{\text{d}E_{\text{dm}}}{1e3}; \quad [\text{kJ/kg}] \]
\[ \text{P}_{\text{fl}}(\text{ct}) = Q; \quad [\text{W}] \]
end;

%% Computing the new properties
\[ \text{ent}_{\text{fl}}(\text{ct}+1) = \text{ent}_{\text{fl}}(\text{ct}) + \text{d}E_{\text{dm}} \text{kJ}; \quad [\text{kJ/kg}] \]
\[ \text{p}_{\text{fl_bar}}(\text{ct}+1) = \left( \frac{\text{p}_{\text{fl_bar}}(\text{ct}) \cdot 1e5 - \text{dp}_{\text{Pa}}}{1e5} \right); \quad [\text{bar}] \]
%% Time and power functions
\[ \text{t}_{\text{total}}(\text{ct}+1) = \text{t}_{\text{total}}(\text{ct}) + \text{dt}; \quad [\text{s}] \]
end;

%% assessing whether mass flows have converged
% Determining new mass flow estimate based on calculated final pressure
% if vaporisation is complete. Otherwise, the computation is senseless
% (non-unity vapour fraction, in compressible fluids)
\[ \text{T}_K = \text{T}_{\text{fl_C}}(\text{ct})+273; \]
if \( x_{\text{vap}}(\text{end}) == 1; \)
    \[ \text{m}_{\text{flow_new}} = C_d \cdot \text{p}_{\text{fl_bar}}(\text{end}) \cdot 1e5 \cdot A_t \cdot VDK / \ldots \]
    \[ (\text{Rs} \cdot \text{T}_K)^{-5}; \quad [\text{kg/s}] \text{ Mass flow through nozzle} \]
% Calculating error
\[ \text{err}_0 = \text{abs}((\text{m}_{\text{flow_new}} - \text{m}_{\text{flow}})/\text{m}_{\text{flow}}); \]
if \( \text{err}_0 > 0.01 \)
    \[ \text{m}_{\text{flow}} = \text{m}_{\text{flow_new}}; \]
    go=1;
else
    go=0;
end;

disp(['Mass flows not yet converged, error is ',num2str(err0*100),'\%'])
disp('Rerunning simulation with updated mass flow')
else
    go=0;
end;

%% calculating nozzle force
if \( x_{\text{vap}}(\text{end}) == 1; \)
    \[ [\text{Pe}_{\text{res}},\ldots] = \text{PressureEvalFun}(\text{p}_{\text{fl_bar}}(\text{end})\cdot 1e5,\gamma; \text{A_ratio},\text{VDK}); \]
    \[ \text{U}_e = \sqrt{2 \cdot \frac{\gamma}{\gamma - 1}} \cdot \text{Rs} \cdot \text{T}_K \cdot \ldots \]
    \[ (1- \left( \frac{\text{Pe}_{\text{res}}}{\text{p}_{\text{fl_bar}}(\text{end})\cdot 1e5} \right)^{((\gamma - 1)/\gamma)}); \]
    \[ \text{F} = \text{m}_{\text{flow_new}} \cdot \text{U}_e \cdot \text{eta}_v + \text{Pe}_{\text{res}} \cdot \text{A_e}; \]
else
    \[ \text{Pe}_{\text{res}} = \text{NaN}; \]
    \[ \text{U}_e = \text{NaN}; \]
    \[ \text{F} = \text{NaN}; \]
end;

end;
end;

% end of calc
\[ \text{F}_{\text{save}}(\text{ct} \_ \text{out}) = \text{F}; \]
\[ \text{m}_{\text{save}}(\text{ct} \_ \text{out}) = \text{m}_{\text{flow_new}}; \]
\[ \text{v}_{\text{save}}(: \_ \text{ct} \_ \text{out}) = \text{v}; \]
\[ \text{tau}(\text{ct} \_ \text{out}) = \text{t}_{\text{total}}(\text{end}); \]
\[ \text{Re}_{\text{save}}(:, \_ \text{ct} \_ \text{out}) = \text{Re}; \]
\[ \text{x}_{\text{vap}_{\text{save}}(:, \_ \text{ct} \_ \text{out})} = \text{x}_{\text{vap}}; \]
P_fl_save(:,ct_out) = P_fl;
p_fl_bar_save(:,ct_out) = p_fl_bar;
T_fl_K_save(:,ct_out) = T_fl_C+273;
T_wall_K_save(:,ct_out) = T_wall_K;
Isp_save(ct_out) = F/m_flow_new/g0;
end;

H.3. **TRANSIENT 1D MODEL**

%% TransientModel_1D.m
% Model designed to assess transient behaviour. The model is used to judge
% assess scenarios that the system would observe during startup and
% operation. Several assumptions are made in this system
% 1. Due to the very high conductivity of silicon, the location of power
  % flux to the fluid does not matter. As such, a reasonable estimate
  % of temperature gradient from wall to liquid suffices to judge the
  % heat per unit of area transfer
% 2. The properties of the liquid do not change throughout the heating
  % process.
% 3. As the main energy requirements stem from the evaporation of the
  % liquid, (liquid heating and evaporation-2.5*10^-6 J/kg versus
  % vapour heating -2*10^-5 J/kg), this is the only process studied.
% 4. As of this evaporation process, the main bulk of energy is added as
  % latent heat, the temperature gradient is assumed to be the
  % difference between heater wall and saturation temperature
% 5. Ideal rocket theory nozzle equations are assumed to have a much
  % faster response than the rest of the system, allowing us to assume
  % that the steady-state formulations can be used without penalty
% 6. Vapour properties (except for density) are assumed constant.
% 7. Vapour properties are assessed at the wall temperature, as the prior
  % example (point 3) showed that the energy needed to raise the vapour
  % to wall temperature is minimal, and steady state models (see
  % SteadyStateModel_1D.m) have shown that this temperature raise
  % occurs very rapidly.
% 8. The transients are based on the Chen et al. [2010] observations, who
  % noticed that often snake-flow would show in the case of too-low
  % wall temperatures. Therefore, the fluid is assumed to maintain the
  % width of the inlet channel (400 um), and flow straight to the exit.
% 9. Balance of in and outflow pressures must be due to evaporation of
  % sufficient fluid, to raise the outlet pressure determined the IGL
  % and the volume available for the vapour.
% File created by C.A.J. Hanselaar for the MSc. thesis project

clear all
% wall temp suggested: 157,167,177,197,297
T_wall_start=177;
T_fluid_in = 20;
p_in_start_bar = 5.5;
Cd_input = 0.7;
pc_input = 1e0;
C_kappa = 1;
%% System input settings
% Implemented to allow external execution of this file based on the pre-set
% wall values T_wall_start (C), fluid input value T_fluid_in (C) and pressure value
% p_start (bar), and prior chamber pressure [Pa]
try
H.3. Transient 1D Model

T_wall_C = T_wall_start; % [C] Wall temperature
T_in_C = T_fluid_in; % [C] Fluid inlet temperature
p_in_bar = p_in_start_bar; % [bar] Fluid inlet pressure
pc = pc_input; % [Pa] a-priori pressure in chamber
Cd = Cd_input; % [1] ejection fraction nozzle

catch
catch(' 
disp(' Sorry Dave, I cannot do that...')
disp(' There is no starting temp or pressure defined, please provide input: ')
disp(' 
T_wall_C = input(' What is the starting wall temperature [C]? ');
T_in_C = input(' What is the starting fluid temperature [C]? ');
p_in_bar = input(' What is the input fluid pressure [bar]? ');
if pc <=0;
disp(' Prior pressure cannot be equal or less than zero,')
disp(' using prior pressure of 1 [Pa] ');
disp(' 
Cd = input(' What is the discharge coefficient for the IRT? ');
disp(' ... '); pause(0.5)
disp(' Thank you, Dave...'); pause(0.5)
disp(' ... ');
end;
T_in_K = T_in_C + 273.15; % [K] Fluid inlet temperature in Kelvin
T_wall_K = T_wall_C + 273.15;% [K] Wall temperature in Kelvin
p_in_Pa = p_in_bar * 1e5; % [Pa] Fluid inlet pressure in Pascal

% Property definitions
% List of pre-determined material properties and other general definitions
% needed for the computation

% Silicon heater properties
k_Si = 149; % [W/(m*K)] Conductivity of silicon base structure
k_g = 1.09; % [W/(m*K)] Conductivity of glass support
em = 0.05; % [1] Emittance factor of exterior

% Fluid properties
Rs = 8314 / 18; % [J/kg/K] Specific gas constant for water
gamma_ideal = 1.3; % [1] specific heat ratio for vapour, assumed constant
VDK = 0.6673; % [1] VanDenKerckhove Function parameter

% general definitions
g0 = 9.81; % [m/s^2] Gravity acceleration
Nu = 6; % [1] Nusselt number estimate based on Bergman2011
T_sat = XSteam('Tsat_p',p_in_Pa); % [C] Saturation temperature

% System dimensions
% Includes all geometric definitions needed to perform the calculations.
% Note that the geometry used is a simplification, assuming no structures
% obstructing the flow, such as the pillars in the design of Poyck and
% Krusharev.

% Heater chamber
H. Analytical Models

L_int = 10e-3; % [m] Interior Length of heater
W_int = 3e-3; % [m] Interior Width of heater
H_int = 0.15e-3; % [m] Exterior Height of heater
A_cs = W_int * H_int; % [m^2] Cross section
Perim = W_int+2 + H_int+2; % [m] Length of perimeter at each cross-section
W_inlet = 0.4e-3; % inlet width
W_L = W_inlet;

% Nozzle structure
W_t = 30.1e-6; % [m] Throat width
A_t = H_int/2 * W_t; % [m^2] Throat area
W_e = 500e-6; % [m] Nozzle exit width
A_e = W_e * H_int; % [m^2] Nozzle exit area
A_ratio = A_e / A_t; % [1] Nozzle expansion ratio

% Exterior dimensions
L_ext = 20e-3; % [m] Exterior Length of heater
W_ext = 10e-3; % [m] Exterior Width of heater
H_ext = 3e-3; % [m] Exterior Height of heater
A_ext = L_ext * W_ext * 2 + H_ext * L_ext * 2 + H_ext * W_ext * 2; % [m^2] Exterior dimensions of the system

% Loop prep
% Starting constants
t = 0; % [s] Simulation time
xL = L_int/100; % [m] Inflow length liquid bulk
xLd = 4; % [m/s] Inflow speed liquid bulk
xLdd = 0; % [m/s^2] Inflow acceleration liquid bulk
rho_V0 = pc / (Rs * T_wall_K); % [kg/m^3] Vapour starting density
L_V = (L_int - xL); % [m] Length of vapour region
m_V = L_V * rho_V0 * W_int * H_int; % [kg] Starting vapour mass

% Permanent constants based on starting constants
my_V = XSteam('my_pT',p_in_bar,T_wall_C); % [Pa * s] Viscosity of vapour, assumed constant
my_L = XSteam('my_pT',p_in_bar,T_in_C); % [Pa * s] Viscosity of liquid, assumed constant
rho_L = XSteam('rho_pT',1,T_in_C); % [kg/m^3] Density of liquid

% Heat transfer properties
DT = T_wall_C - (1*T_sat+0*T_in_C); % [C] Temperature differential wall to liquid
kappa = C_kappa *XSteam('tc_pT',1,20); % [W/m/K] Thermal conductivity of liquid

cp_evap = 2.2e6 + (T_sat-T_in_C)*4.2e3; % [J/kg] Energy per kg for evaporation

% Loop start
go=1; % [1] Boolean variable
c=s; % [1] Counter variable
save_count = NaN; % [1] Error reporting variable
dt = 1e-6; % [s] Time step for loop

while go==1;

% Masses
% present liquid mass
\[ m_L(\text{ct}) = W_L \cdot H_{int} \cdot \rho_L \cdot (x_L(\text{ct})); \]

% mass flows (out through nozzle, in via evaporation)
\[ m_{out}(\text{ct}) = C_d \cdot \rho_c(\text{ct}) \cdot V_{DK} \cdot A_t / \sqrt{R_s \cdot T_{wall_K}} \text{ [kg/s]} \]
\[ \text{Power}(\text{ct}) = (DT \cdot \kappa / H_{int} \cdot (2 \cdot W_L \cdot x_L(\text{ct}))); \]
\[ m_{evap}(\text{ct}) = \text{Power}(\text{ct}) / (\rho_{evap}); \text{ [kg/s]} \]

%% Force balance on liquid
% Force based on pressure difference input and nozzle plus vapour
% gradient
\[ F_p(\text{ct}) = (p_{in_Pa} - p_c(\text{ct}) \cdot W_L \cdot H_{int}; \]
% Force based on viscous forces on liquid
\[ F_{my_L}(\text{ct}) = 12 \cdot m_y_L \cdot x_{Ld}(\text{ct}) \cdot x_L(\text{ct}) / H_{int}^2 \cdot (W_L \cdot H_{int}); \]
% Summation of forces
\[ F_{sum}(\text{ct}) = F_p(\text{ct}) - F_{my_L}(\text{ct}); \text{ [N]} \]

%% Acc, spd, pos
% Acceleration term of liquid
\[ x_{Ldd}(\text{ct+1}) = (F_{sum}(\text{ct}) / (2 \cdot W_L \cdot H_{int} \cdot \rho_L) - x_{Ld}(\text{ct})^2) / x_L(\text{ct}); \text{ [m/s}^2\text{]} \]
% Integration to speed of liquid front
\[ x_{Ld}(\text{ct+1}) = x_{Ld}(\text{ct+1}) * dt; \]
% correcting front speed for the evaporated liquid
\[ m_{evap_corr} = m_{evap}(\text{ct}) / (W_L \cdot H_{int} \cdot \rho_L) \cdot dt; \]
\[ x_{Ld}(\text{ct+1}) = x_{Ld}(\text{ct}) - m_{evap_corr}; \]
% Integration to liquid front position
\[ x_L(\text{ct+1}) = x_L(\text{ct}) + x_{Ld}(\text{ct+1}) * dt; \]

%% Correcting for out-of-domain settings
if \[ x_L(\text{ct+1}) < L_{int}/400 \]
\[ x_L(\text{ct+1}) = L_{int}/400; \]
if \[ x_Ld(\text{ct+1}) < 0 \]
\[ x_Ld(\text{ct+1}) = 0; \]
end;
if \[ x_Ldd(\text{ct+1}) < 0 \]
\[ x_Ldd(\text{ct+1}) = 0; \]
end;
\[ m_{evap}(\text{ct}) = 0; \text{ [kg/s]} \text{ setting evaporation speed to zero}\]
% keeping track of the first occurance
\[ \text{save_count2} = \text{save_count}, \text{ct}; \]
\[ \text{save_count} = \text{min(save_count2)}; \]
end;

%% Vapour calculations
% Remaining vapour length
\[ L_V(\text{ct+1}) = L_{int} - x_L(\text{ct+1}); \text{ [m]} \]
\[ V_{ol_V} = W_{int} \cdot H_{int} \cdot L_{int} - x_L(\text{ct+1}) \cdot W_L \cdot H_{int}; \]
% Vapour mass
\[ m_V(\text{ct+1}) = m_V(\text{ct}) + (m_{evap}(\text{ct}) - m_{out}(\text{ct})) \cdot dt; \text{ [kg]} \]
% Average vapour pressure
\[ p_{V_avg}(\text{ct+1}) = m_V(\text{ct+1}) / \text{(Vol}_V) \cdot R_s \cdot T_{wall_K}; \text{ [Pa]} \]
% Nozzle pressure using the average pressure and fixed gradient
\[ p_c(\text{ct+1}) = p_{V_avg}(\text{ct+1}); \]

%% timing and quitting
\[ t(\text{ct+1}) = t(\text{ct}) + dt; \]
if \( x_L(\text{ct}+1) > L_{\text{int}} \times 0.99 \)
go = 0;
disp('Liquid entering nozzle, quitting')
elseif \( x_L(\text{ct}+1) < L_{\text{int}} / 800 \)
go = 0;
disp('Liquid leaving chamber through inlet, quitting')
\% Should be impossible due to out-of-domain corrections, kept in
\% place to prevent otherwise strange errors
elseif \( t(\text{ct}+1) > 1.2 \)
go = 0;
disp('Maximum time superceded, quitting')
end;

\text{ct} = \text{ct} + 1;
end;
\%
Reporting on possible errors due to liquid being forced back too much,
\% and corrections occurring. A stable simulation might still be completed,
\% but the dynamics have been truncated.
if isnan(save\_count)
else
    disp('')
disp(['Starting at iteration number ',num2str(save\_count),','])
disp([' corresponding to time ', num2str(t(save\_count)), '[s],'])
disp(' the inflow distance was lower than the minimal length,')
disp(' so it was increased until minimal length was reached.'))
disp('')
end;