Hierarchical two-phase flow models for autonomous control of cryogenic loading operation

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Abstract. We report on the development of a hierarchy of models of cryogenic two-phase flow motivated by NASA plans to develop and maturate technology of cryogenic propellant loading on the ground and in space. The solution of this problem requires models that are fast and accurate enough to identify flow conditions, detect faults, and to propose optimal recovery strategy. The hierarchy of models described in this presentation is ranging from homogeneous moving-front approximation to separated non-equilibrium two-phase cryogenic flow. We compare model predictions with experimental data and discuss possible application of these models to on-line integrated health management and control of cryogenic loading operation.

1. Introduction
The human exploration beyond low Earth orbit requires development of a new suite of cryogenic fluid management technologies [1, 2] including autonomous cryogens transfer and settling, active thermal control and positioning of cryogens in the tanks, on-line health management and control. As an important step towards future sustainable and reliable space exploration NASA is developing and maturating technologies and advanced cryogenic hardware for autonomous integrated health management (IHM) and control of ground launch operations [3].

One of the challenging problems in this development is fast and reliable predictions of the two-phase cryogenic flow [4]. Despite recent progress [5, 6, 7, 8] the state of the art in two-phase modeling exhibits a lack of general agreement regarding the fundamental physical models that describe the complex phenomena [8] and a wide diversity of algorithms [5, 6, 7, 9] developed for integration of these models. One of the major problems (see, however, recent claims [8]) is a large number of instabilities inherent to these solvers [7, 10, 11].

These solvers heavily rely on a large number of correlations developed for boiling two-phase flows (see e.g. [12, 6]). However, knowledge of these correlations for cryogenic flows remains sparse [13]. Even less is known about flow boiling correlations of cryogenic fluids in micro-gravity [14, 15]. To mitigate this problem the future model-based IHM system has to be intelligent enough to create and extend database of required correlations and to learn continuously missing information.
It was proposed in our earlier work [4] that an efficient approach to the integrated health management and control of cryogenic flows can be based on a hierarchy of two-phase flow models. We have coded and tested a number of solvers for this hierarchy that include quasi-steady homogeneous moving front [16, 17], semi-implicit and nearly-implicit [4] solvers for homogeneous and separated cryogenic flow.

The choice of the models in the hierarchy is motivated by the solution of the speed-accuracy trade-off problem that provides fast predictions with required fidelity for a wide range of flow regimes. It is also important to ensure that all the models in the hierarchy are suitable for on-line IHM and control oriented applications (see e.g. [5, 6, 18, 19]) and can be applied to the off- and on-line optimization and learning of cryogenic flow parameter.

Here we report on the progress in development and validation of such models. First, we briefly describe two key components of the hierarchy – separated and homogeneous models of the flow. Next, we discuss validation of these models using experimental data obtained at the cryogenic transfer line build at NASA Kennedy Space Center (KSC). In Section 4, we provide some preliminary results on the parameter estimation and optimization. Finally, we formulate some conclusions and discuss future work.

2. Models of the cryogenic two-phase flow

In developing fast on-line control-oriented applications we limit our analysis to one-dimensional two-phase flow models. The hierarchy of models [4] included in our study consists of single-phase isothermal flow, moving front variation of the homogeneous model (HM), and two-fluid separated model (SM). The hierarchy extends through the whole range of approximations currently used to model 1D flow networks and allows to use a trade-off between the accuracy and complexity/speed of the solution whenever required. Here we briefly describe some results obtained for the SM model. The best studied model of this type is the Wallis [20] one-pressure model. This model consists of a set of mass, momentum, and energy conservation laws written for each phase.

2.1. Separated model

Let us consider control volume of a pipe of length $L$ and cross-section area $A$. The geometry of the flow in this control volume is characterized by the wetted ($l_wl$), dry ($l_wg$), and interface ($l_i$) perimeters and by the angle $\theta$ of the pipe axis with respect to the horizontal line. For the separated model of the two-phase cryogenic flow the conservation equations for each phase take the following form

$$
\begin{align}
(\alpha \rho g)_{,t} + \frac{1}{A} (A \alpha \rho g u_g)_{,x} &= \Gamma_g; \\
(\beta \rho i)_{,t} + \frac{1}{A} (A \beta \rho i u_i)_{,x} &= -\Gamma_g
\end{align}
$$

(1)

for the mass

$$
\begin{align}
(\alpha \rho_g u_g)_{,t} + \frac{1}{A} (A \alpha \rho_g u_g^2)_{,x} + \alpha p_{,x} &= -\alpha \rho_g \sin \theta - \tau_{wg} \frac{l_wg}{A} - \tau_{ig} \frac{l_i}{A} + \Gamma_g u_{ig}; \\
(\beta \rho_i u_i)_{,t} + \frac{1}{A} (A \beta \rho_i u_i^2)_{,x} + \beta p_{,x} &= -\beta \rho_i \sin \theta - \tau_{wl} \frac{l_{wl}}{A} - \tau_{il} l_i - \Gamma_g \frac{u_{ig}}{A}
\end{align}
$$

(2)

the momenta

$$
\begin{align}
(\alpha \rho_g e_g)_{,t} + \frac{1}{A} (A \alpha \rho_g e_g u_g)_{,x} &= -\frac{1}{A} (pA \alpha u_g +)_{,x} \alpha p_{,x} + \dot{q}_{wg} \frac{l_wg}{A} + \dot{q}_{ig} \frac{l_i}{A} + \Gamma_g h_{ig} + \Gamma_g h_{wg}; \\
(\beta e_i u_i)_{,t} + \frac{1}{A} (A \beta e_i u_i u_i)_{,x} &= -\frac{1}{A} (pA \beta u_i +)_{,x} \beta p_{,x} + \dot{q}_{wl} \frac{l_{wl}}{A} + \dot{q}_{il} \frac{l_i}{A} - \Gamma_g h_{ig} - \Gamma_g h_{wg}
\end{align}
$$

(3)

and for the energy.
Each phase is characterized by the void fraction $\alpha_k$, density $\rho_k$, temperature $T_k$ (energy $e_k$), and velocity $u_k$, where index $k$ is $g$ for the gas/vapor phase and $k$ is $l$ for liquid phase. Here $\Gamma_g$ is the interfacial mass flow rate, $\dot{q}_{gw}$, $\dot{q}_{lw}$, and $\dot{q}_{ki}$ are heat fluxes to the dry wall and wetted walls, and to the interface. Pressure losses at the dry, wetted wall, and interface are $\tau_{(gw)}$, $\tau_{(lw)}$, and $\tau_{ki}$ respectively. The relative velocity at the interface is $u_{ik}$.

The set of equations (1) - (3) is completed by adding volume conservation condition and equations of state for each phase

$$\alpha_g + \alpha_l = 1, \quad \rho_{(g,l)} = \rho_{(g,l)} \left( p, e_{(g,l)} \right)$$

(4)

The fluid dynamics equations (1) - (4) are thermodynamically coupled to the equation for energy conservation for the unit length of the wall

$$\rho_w c_w d_w \frac{\partial T_w}{\partial t} = H_{wg} (T_g - T_w) + H_{wl} (T_l - T_w) + H_{amb} (T_{amb} - T_w).$$

(5)

The heat transfer to the wall is characterized by the heat transfer coefficient from gas (liquid) to the wall $H_{g(l)w}$ and the heat transfer coefficient from the environment to the wall $H_{amb}$. $T_w$ is the wall temperature, and $\rho_w$, $c_w$, and $A_w$ are wall material density, specific heat, and cross-section area.

In the SM the source terms are calculated using heat transfer and pressure losses correlations based on flow pattern recognition. At present, the model can recognize horizontally stratified, annular, and dispersed flow regimes using the flow map introduced for refrigerants by Wojtan et al [21].

The single phase friction factor $f_{g(l)}$ is approximated using the Churchill formula [22]. The two-phase friction pressure drop is defined using the Lockhart-Martinelli correlations [23].

The heat transfer coefficients at the wall ($H_{g(l)w}$) and at the interface ($H_{g(l)i}$) are defined by a large set of correlations that depend on the flow patterns. For example, for horizontally stratified regime corrected pool boiling correlations are used to estimate convective, nucleate boiling, transition boiling, and film boiling heat transfer. In other flow regimes the analysis of correlations follows results obtained in [6, 5] and the details will be provided elsewhere.

It is assumed in these correlations that local pressures for each phase are equal ($p_g = p_l = p$) and that the source terms in eqs. (1) - (3) are exclusively algebraic functions of state and flow parameters. These assumptions reflect the incomplete current knowledge of the interaction of the phases with the wall and with each other. As a consequence the SM is known to display a number of instabilities that can slow down and sometimes prevent convergence of the solver.

In particular, this model is known to be non-hyperbolic [9, 24], to display lack of positivity [11] and instabilities due to phase appearance and disappearance [7, 11]. In addition, this model represents a system of “stiff” differential equations [9].

Although a large number of techniques exists that reduce the effect of instabilities the problem cannot be eliminated completely. One of the ways to mitigate it is to use a hierarchy of models where a more robust lower fidelity model can guarantee uninterrupted performance of the system as whole. An extensive numerical testing revealed that this can be done e.g. by adding to the hierarchy homogeneous moving-boundary quasi-steady model of two-phase cryogenic flow [16, 17] as will be discussed below.

2.2. Homogeneous moving front model

The homogeneous model of the two-phase flow can be obtained from the SM by summing pairwise conservation equations (1), (2), and (3) under the assumption that in the two-phase region both
phases have the same temperature \((T = T_g = T_l)\) and velocity \((u = u_g = u_l)\)

\[
\rho, + (\rho u)_z = 0, \\
(\rho u)_t + (\rho u^2)_z = -p_z - \frac{1}{A}(\tau_w l_w)_{2\phi} - \rho g \sin \theta, \\
(\rho e)_t + (\rho u h)_z = \frac{1}{A} \dot{q}_w l_w.
\]  

These equations are written in terms of the mixture density \(\rho\) and enthalpy \(h\)

\[
\rho = \alpha \rho_v + (1 - \alpha) \rho_l; \quad h = x h_v + (1 - x) h_l
\]

The moving-boundary version of the HM model [18] allows one to use linear approximation for the mass fraction in the two-phase region and to incorporate up to three coexisting states of the fluid (vapor, liquid, and their mixture) within one control volume, therefore, increasing fidelity of the model.

To speed up integration of the model [16, 17] the momentum equation is solved in the quasi-steady approximation, neglecting inertia terms \((\cdot)_z\) denote spatial derivative)

\[
(Apu^2)_{z} = -\frac{1}{A} (\tau_w l_w)_{2\phi} - p_z - \rho g \sin \theta.
\]  

In this approach calculations of the mass fluxes is decoupled from the integration of the conservation equations for the mass and energy. The resulting algorithm allows for very fast and time-accurate predictions of the cryogenic two-phase flow in transfer lines.

An additional acceleration of the integration of homogeneous model is achieved by using a much smaller set of correlations as compared to the correlations used by the SM. In the HM the single phase frictional losses were calculated using the Swami-Jain [25] approximated solution of the Colebrook approximation. For the two-phase flow the frictional losses were calculated according to the Mueller-Steinhagen and Heck correlation [25]. The Dittus-Boelter approximation with the Gungor-Winterton boiling enhancement factor [25] was used to calculate the heat transfer.

2.3. Solution algorithms

The nearly-implicit solution algorithm developed for the SM follows closely the ideas of [6] and is described in more detail in [26]. It was designed to break time step restrictions imposed by the acoustic and material Courant-Friedrichs-Lewy condition.

The solution of the linearized on staggered grid set of equations is performed in two steps. The first step, structured as a predictor of the fractional time step technique, can be briefly summarized as follows: (i) Solve expanded equation with respect to pressure in terms of new velocities; (ii) Solve momenta equations written in the form of block tri-diagonal matrix for the new velocities; (iii) Find new pressure; (iv) Find provisional values for energies and void fractions using expanded equations; (v) Find provisional values of mass fluxes and heat transfer coefficients using provisional values of temperatures obtained.

At the second step new (corrected) values of the densities, void fractions, and energies are calculated by solving the unexpanded conservation equations for the phasic masses and energies using provisional values for the heat and mass fluxes in source terms.

To mitigate the instability problem we use a number of techniques including staggered grid, upwinding, virtual mass, limiters on the values of pressure, active time step control and smoothers that control phase appearance/disappearance.

The resulting algorithm is quite reliable and fast, it scales linearly with the number of control volumes, and yet it resolves both acoustic and material waves [27] in the system.
The integration of the HM is described in details in [16]. The solution of the HM was substantially sped up by using quasi-steady approximation [16] that allows to decouple calculations of the mass fluxes from the integration of the conservation equations for the mass and energy. The resulting algorithm is using only the two first sub-steps of the SM algorithm described above and explicit Euler time stepping. It allows for very fast and time-accurate predictions of cryogenic two-phase flow in transfer lines.

3. Validation
Both models were extensively verified using a number of numerical tests [17, 27] and comparison with results obtained using SINDA/FLUINT model of the transfer line [28]. The models were validated by comparison with real data obtained during chilldown of a cryogenic transfer at National Bureau of Standards (NBS) [29] and those from the cryo-testbed at KSC [3].

In the NBS experiment the vacuum jacketed line was 61 m long. The internal diameter of the copper pipe was 0.02 m. Four measurement stations were located at the distance 6, 24, 42, and 60 m from the input valve. The working liquid was nitrogen and pressure in the storage tank was 4.2 atm, while the other end of the pipe was opened to the atmosphere.

The KSC cryo-testbed consists of a storage tank and an external tank connected by a pipeline. A number of control valves and sensors are located along the lines. The cryogenic fluid is nitrogen. The total length of the line is \( \sim 45 \) m. The characteristic transient time of the pressure equilibration is less than 1 sec. The diameter \( D \) of the stainless steel pipe varies along the line. The thickness \( d_w \) of the walls is approximately 3 mm.

An example of the HM validation using the KSC data is shown in Fig. 1. It can be seen from the figure that the model can accurately reproduce the main dynamical features observed experimentally for both pressure and temperature. Similar results were obtained for the SM. It is important to note that the integration time for both models is quite small. For example, simulations of the 1.5 hours of real loading time using the SM takes \( \sim 10 \) sec on a laptop. The HM performs the same simulations in \( \sim 1 \) sec.

![Figure 1. The results of the validation of the homogeneous model using experimental data obtained at the KSC testbed. The model predictions (dashed lines) of the chilldown in cryogenic transfer line are shown in comparison with experimental data (solid lines): (top) temperature and (bottom) pressure at three locations along the pipeline.](image-url)
cryogenic flow in transfer lines by these models pave the way to the development of model-based on-line control-oriented applications and intelligent integrated health management.

4. Parameter estimation

As a first step towards intelligent on-line health management and control we are currently developing a set of model-based optimization tools that would allow one to infer and learn unknown parameters of the flow, evaluate faults in the transfer line, optimize the design of the transfer lines, optimize flow regimes and fault recovery strategies.

This development is performed in a number of stages taking into account the fact that many model parameters are poorly known and the cost function associated with this set of parameters has a very complex landscape with multiple local minima and non-trivial trade-offs.

First, we perform an extensive parametric sensitivity studies of the model responses to determine a subset of the most important parameters. Next, we develop a number of optimization tools (including e.g. direct search, unconstrained nonlinear optimization, and Markov Chain Monte Carlo) to infer the values of parameters that correspond to the best fit to the available experimental data. To continuously learn model parameters from the extended databases of experimental data we are planning to develop model-based machine learning algorithms.

For example, the sensitivity study for the NBS model, which involved analysis of over 30 correlation parameters, revealed that only ~ 10 of them can significantly change the model dynamics. The outcome of the sensitivity studies for one of these parameters is shown in Fig. 2. The top figure shows model predictions for the fluid temperature as compared to the experimental time-traces. The bottom figure shows similar comparison for the heat transfer coefficient. The results of this example demonstrate that scaling heat transfer coefficient by 10% can change cost function by 30% emphasizing significance of this parameter.

It can be seen from the figure that the model can quite accurately reproduce experimental data including a sudden temperature drop that occurs as the wall cools down to approximately

![Figure 2](image_url)

**Figure 2.** Model predictions (dashed lines) for the fluid temperature (top) and heat transfer coefficient (bottom) are shown in comparison with the experimental time-traces (solid lines with open symbols) at 4 locations from the pipeline entrance: (i) 6 m (open circles); (ii) 24 m (open squares); (iii) 42 m (open diamonds); and (iv) 60 m (open triangles). Different dashed lines correspond to 9 different values of the heat transfer coefficient.
Figure 3. Results of application of unconstrained nonlinear optimization illustrating evaluation of the off-nominal value of model parameter. (a) - (b) show the deviation of the temperature and pressure sensors data (solid lines with open circles) from the nominal regime (solid lines with open squares) beyond the margins (dashed lines). (c) shows the convergence of the cost function to its minimum vs the number of iterations. (d) shows the convergence of the model parameter to its target value corresponding to 10% leak in the pipe section.

130 K corresponding to the transition from the film boiling regime to the intermittent regime of boiling.

To evaluate parameters that provide the best fit of the model predictions to the measured data we are developing a set of optimization tools. An application of one of such tools for evaluation of parameters of homogeneous model is illustrated in the Fig. 3. In this example we infer off-nominal value of the model parameter that represents fault. The measured time-traces corresponding to the off-nominal dynamics were simulated by injecting a 10% gas leak fault at the middle of the transfer line at $t = 0$ sec. The time traces corresponding to the nominal and off-nominal operation are shown in the Fig. 3.

In the test the deviation of the “measured” time-traces from the nominal regime beyond the margins (see Fig. 3 (b)) signals fault detection. Once the fault was detected the system invokes unconstrained nonlinear optimization tool to evaluate the fault. The initial value of the parameter, which is the diameter of a hole in the pipe wall, is 0 (nominal).

The cost function was chosen as a sum of squared difference between the measured and predicted data for the pressure and temperature sensors along the transfer line. The summation was performed over $N_f$ time steps, where $N_f = t_f/\Delta t$, $t_f = 200$ sec is the characteristic time scale of the fault evolution and $\Delta t$ is the discretization time. It can be seen from the figure that the optimization procedure converges to the correct value of the fault parameter after $\sim 20$ iterations. Each iteration takes less than 0.5 sec and the convergence occurs in less than 10 sec.

5. Conclusions
In conclusion, it was shown that fast and accurate predictions of the two-phase cryogenic flows can be obtained using a hierarchy of models ranging from quasi-steady homogeneous model to separated non-equilibrium model of the flow. We demonstrated application of these models to the estimation and evaluation of the model parameters using optimization algorithms.

The fast and robust performance of the models allows one to develop a set of optimization tools capable of on-line and off-line evaluation of the model parameters. These results pave the way to the development of the model-based integrated health management and control of the
cryogenic systems.
In the future we will demonstrate an application of this approach to the model-based fault detection, isolation and recovery in the cryogenic transfer line. As a more distant application of this approach we are currently studying the feasibility of development model-based intelligent IHM of cryogenic systems that will allow to create and extend databases for cryogenic correlations and faults and infer missing information.

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