Inferential framework for autonomous cryogenic loading operations

Dmitry G Luchinskiy¹, Michael Khasin², Dogan Timucin³, Jarred Sass⁴, Jose Perotti⁵, Barbara Brown⁶

^{1,2} SGT, Inc., Greenbelt, MD, USA dmitry.g.luchinsky@nasa.gov michael.khasin@nasa.gov

³ NASA Ames Research Center, Moffett Field, CA, 94035, USA dogan.timucin@nasa.gov

^{4,5,6} Kennedy Space Center, Kennedy Space Center, FL, 32899, USA jose.m.perotti@nasa.gov jared.p.sass@nasa.gov barbara.l.brown@nasa.gov

ABSTRACT

We address the problem of autonomous cryogenic management of loading operations on the ground and in space. As a step towards the solution of this problem we develop a probabilistic framework for inferring correlations parameters of two-fluid cryogenic flow. The simulation of two-phase cryogenic flow is performed using nearly-implicit scheme. A concise set of cryogenic correlations is introduced. The proposed approach is applied to an analysis of the cryogenic flow in experimental Propellant Loading System built at NASA Kennedy Space Center. An efficient simultaneous optimization of a large number of model parameters is demonstrated and a good agreement with the experimental data is obtained.

1. INTRODUCTION

NASA program of advanced cryogenic loading operations is focused on development of technologies enabling effective space exploration (Chato, 2008; Notardonato, 2012; Konishi & Mudawar, 2015a). These technologies require models that can recognize and predict cryogenic fluid regimes without human interaction. The accuracy of these predictions depends largely on the functional form and parameterization of correlations for the flow patterns, pressure losses, and the heat transfer in cryogenic fluids. However, knowledge of these correlations remains limited and their learning presents significant challenge to scientists and engineers (Tong & Tang, 1997; Faghri & Zhang, 2006; Ghiaasiaan, 2007; Konishi & Mudawar, 2015b). This problem becomes even more challenging for applications in microgravity (S. R. Darr et al., 2016a, 2016b).

Research conducted to address this and other critical issues of space exploration resulted in a number of important achievements, see e.g. (Konishi & Mudawar, 2015a; S. R. Darr et al., 2015; Hartwig & Vera, 2015; Hedayatpour, Antar, & Kawaji, 1990; Kawaji, 1996; A. Majumdar & Steadman, 2003; A. K. Majumdar & Ravindran, 2010; Yuan, Ji, & Chung, 2007, 2009; Chung & Yuan, 2015; S. Darr et al., 2016; S. R. Darr et al., 2016a, 2016b) and references therein. Specifically, a number of optimization techniques have become available for analysis of the model parameters and data correlations (Cullimore, 1998).

However, small time steps and instabilities of numerical schemes impose substantial limitations on the speed of the twofluid cryogenic codes and possibility of their on-line applications in autonomous systems. As a result accurate predictions of transient cryogenic flows and optimization of the parameters of cryogenic systems remain a challenge (Hartwig & Vera, 2015; Cullimore, 1998; Konishi & Mudawar, 2015a; S. R. Darr et al., 2015).

Here we report on progress in the development of probabilistic framework capable of efficient multi-parametric inference of cryogenic correlations and accurate predictions of experimental time-series data.

The paper is organized as follows. In the following section we briefly describe model equations and method of their integration. In Sec. 3 we discuss correlation relations for two-phase cryogenic fluid. In Sec. 4 we introduce probabilistic frame-

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work for multi-parametric inference of the model parameters. An application of the inferential framework to the analysis of cryogenic flow in experimental Propellant Loading System is discussed in Sec. 5. Finally, in Conclusions we summarize the obtained results and discuss future applications.

2. MODEL

2.1. Model equations

The system is divided into a set of coupled control volumes. In each control volume the flow is modeled using six conservation equations for gas (vapor) and liquid phases (D. G. Luchinsky, Smelyanskiy, & Brown, 2014a, 2014c, 2014b; D. G. Luchinsky et al., 2016), see also (Luchinskiy et al., 2015; D. G. Luchinsky et al., 2015). The following set of equations used

$$\frac{\partial}{\partial t} \begin{bmatrix} \alpha \rho \\ \alpha \rho u \\ \alpha \rho e \end{bmatrix}_{j}^{+} + \frac{\partial}{\partial t} \begin{bmatrix} \alpha \rho u \\ \alpha \rho u^{2} \\ \alpha \rho e u \end{bmatrix}_{j}^{-} = \begin{bmatrix} 0 \\ p \left(s \alpha_{,t} - (\alpha u)_{,x} \right) \end{bmatrix}_{j}^{-} , \quad (1) + \begin{bmatrix} s_{j} \Gamma \\ \alpha \rho z_{,x} - \tau_{w} l_{w} - \tau_{i} l_{i} + \Gamma u_{i} \\ \dot{q}_{w} \frac{l_{w}}{A} + \dot{q}_{i} \frac{l_{i}}{A} + \Gamma h_{i} \end{bmatrix}_{j}^{-}$$

where j takes values g for the gas and l for the liquid. The dynamical variables in this system are: void fraction α (volume conservation requires $\alpha_g + \alpha_l = 1$), pressure p, phasic densities $\rho_{g(l)}$, velocities $u_{g(l)}$, and thermal energies $e_{g(l)}$. The variable s_j takes value -1 for the liquid and +1 for the gas. The system (1) is closed by adding constitutive relations and equations of states. The equations of states are implemented in the form of tables. The values of the heat (\dot{q}) and mass (Γ) fluxes at the wall and interface (subscripts w and i correspondingly) are given by correlation relations.

The system (1) is coupled to the energy conservation equation for the pipe wall in each control volume

$$\rho_w c_w d_w \frac{\partial T_w}{\partial t} = h_{wg} \left(T_g - T_w \right) + h_{wl} \left(T_l - T_w \right) + h_{amb} \left(T_{amb} - T_w \right).$$
(2)

Here T_w is the pipe wall temperature, ρ_w , c_w , and d_w are density, specific heat, and thickness of the pipe wall, h is the heat transfer coefficient corresponding to the ambient (h_{amb}) and internal heat flowing to the wall from the gas (h_{wg}) and liquid (h_{wl}) phases.

The total mass transfer Γ_g in equations (1) is the sum of the mass transfer at the wall (w) and at the interface (i)

$$\Gamma_g = \Gamma_{wg} + \Gamma_{ig},$$

where

and

$$H_{g}^{*} - H_{l}^{*} = \begin{cases} H_{g,s} - H_{l}, & \Gamma > 0\\ H_{g} - H_{l,s}, & \Gamma < 0 \end{cases}$$

 $\Gamma_{wg} = \frac{\dot{q}_{wl}}{H_g^* - H_l^*}; \qquad \Gamma_{ig} = \frac{\dot{q}_{li} + \dot{q}_{gi}}{H_g^* - H_l^*};$

The heat fluxes at the wall and at the interface are

$$\begin{split} \dot{q}_{wg} &= h_{wg} \left(T_w - T_g \right); \quad \dot{q}_{ig} = h_{ig} \left(T_{l,s} - T_g \right); \\ \dot{q}_{wl} &= h_{wl} \left(T_w - T_l \right); \quad \dot{q}_{il} = h_{il} \left(T_{l,s} - T_l \right). \end{split}$$

Here $T_{l,s}$ is the saturation temperature of the liquid.

2.2. Algorithm

The integration of the model (1) - (2) was performed in two steps following closely the nearly-implicit method described in RELAP5-3D (RELAP5-3D-I, 2012), see (D. G. Luchinsky et al., 2014c; Luchinskiy et al., 2015) for the details. The first step of the algorithm can be briefly summarized as follows: (i) Solve the set of coupled expanded density-energy equations 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 values of the densities, void fractions, and energies are found by solving the unexpanded conservation equations for the phasic masses and energies. Provisional values for the heat and mass fluxes in the source terms are used at this step. The solution is reduced to independent solution of four tri-diagonal matrices. Values of the pressure and velocities in these matrices are taken at the new time step.

The resulting computational scheme is efficient and fast and can integrate 1000 sec of real time chilldown in a few seconds of computational time. For a model consisting of N control volumes it involves inversion of N 4 × 4 matrices, solution of $2 \times (N-1)$ tree-block-diagonal matrix equation, solution of four $N \times N$ tridiagonal matrix equations, and $N \times m$ explicit computations.

A major difficulty in practical implementation of this scheme is related to several numerical instabilities. The mitigation of known stability issues in our algorithm is discussed in (D. G. Luchinsky et al., 2014a, 2014c, 2014b, 2016; Luchinskiy et al., 2015; D. G. Luchinsky et al., 2015)

3. CONSTITUTIVE RELATIONS

The model equations introduced above have to be closed using the equations of state and the constitutive relations. The equations of state can be included into the model in the form of NIST tables (Lemmon, Huber, & McLinden, 2013; D. G. Luchinsky et al., 2014c).

Functional and parametric form of the constitutive relations, on the other hand, represent one of the main source of uncertainties in the model. In this work we use constitutive relations (D. G. Luchinsky et al., 2016) based on the recognition of the flow boiling regimes and for each regime we define interphase friction, the coefficient of virtual mass, wall friction, wall heat transfer, interphase heat and mass transfer.

First, the boundaries between flow boiling regimes are determined at each time step. Next, the flow correlations are defined for each flow regime.

The boundaries between flow regimes are estimated using simplified Wojtan et al (Wojtan, Ursenbacher, & Thome, 2005) map. The map was simplified in two ways. First, we used only three transition boundaries. Next, we estimated the location of these boundaries in the coordinates of mass flow rate (\dot{m}) and vapor quality (χ) using original expressions. Finally, we approximated the location of these boundaries and used polynomial coefficients as fitting parameters.

The rationale behind the approximated description of the boundaries of the flow regimes is twofold. It is known (Jackson, 2006) that Wojtan maps can only be considered as an approximation to the flow regimes of cryogenic fluids. In the experiments performed at KSC the flow regimes were not established experimentally and therefore cannot be validated.

The following transitions between flow regimes were included into correlations: (i) Stratified-Wavy-to-stratified transition; (ii) Stratified-Wavy-to-annular-intermittent transition; and (iii) Dryout transition.

3.1. Heat and mass transfer

In the current work we are interested in the relatively low mass fluxes, $G < 600 kg/m^2/s$. In this limit correlations for the heat flux are often based on the multiplicative or additive corrections to the values obtained for the pool boiling (Franchello, 1993; Seader, Miller, , & Kalvinskas, 1965; Griffith, 1957; Zuber & Tribus, 1958; Kutateladze, 1959). The following heat transfer mechanisms are included in the analysis: (i) convection, (ii) nucleate boiling, (iii) transition boiling, (iv) film boiling, and (v) transition to dryout regime.

3.1.1. Convective Heat Transfer

Convective heat transfer in horizontal pipes distinguishes four flow regimes: forced laminar, forced turbulent, natural laminar, and natural turbulent convection. The corresponding correlations for the convective heat transfer can be taken in the form e.g. (TRACE-V5.0, 2007; RELAP5-3D-IV, 2012; Nellis & Klein, 2009; Holman, 1989)

$$h_{cb} = \frac{\kappa}{D_h} \begin{cases} 4.36, & \text{Forced-Laminar;} \\ 0.023 \cdot Re^{0.8} Pr^{0.4}, & \text{Forced-Turbulent;} \\ 0.1 \cdot (Gr \cdot Pr)^{1/3}, & \text{Natural-Laminar;} \\ 0.59 \cdot (Gr \cdot Pr)^{1/4}, & \text{Natural-Turbulent.} \end{cases}$$
(3)

Here $Pr = \frac{\mu C_p}{\kappa}$ and $Gr = \frac{\rho^2 g \beta_T (T_w - T_{l(g)}) D^3}{\mu^2}$ are Prandtl and Grashof numbers respectively, β_T is the coefficient of thermal expansion, and D_h is the hydraulic diameter. To guarantee a smooth transition between various regimes the maximum value of h_{cb} is taken as the value for the convective heat transfer.

We note that convective heat transfer in the stratified flow does not significantly affect the chilldown process, because the fluid temperature in this regime is close to (or lower than) saturation temperature T_s . The first critical temperature that defines the shape of the boiling curve and influences the chilldown corresponds to the onset of nucleation boiling T_{onb} .

3.1.2. Onset of nucleate boiling

The correlations for temperature T_{onb} and the corresponding heat flux \dot{q}_{onb} for onset of nucleate boiling can be written (Sato & Matsumura, 1964; Frost & Dzakowic, 1967; Ghiaasiaan, 2007; Huang, 2009) as

$$T_{onb} = T_s + F\left(1 + \sqrt{1 + \frac{2\Delta T_{sub}}{F}}\right), \qquad (4)$$

$$\dot{q}_{onb} = \frac{B}{Pr^2} \Delta T_{sat}^2 = h_{cb} (T_{onb} - T_l)$$
(5)

where $B = \frac{\rho_g h_{lg} \kappa_l}{8\sigma T_s}$, $F = \frac{h_{cb} P r_l^2}{2B}$, $\Delta T_{sat} = T_{onb} - T_s$ is the wall superheat, and $\Delta T_{sub} = T_s - T_l$ is liquid subcooling temperature. The convective heat transfer coefficient in the Eq. (5) is given by Eq. (3).

When the wall temperature is increased the heat flux to the wall may increase by more than an order of magnitude until the heat flux approaches its critical value \dot{q}_{chf} .

3.1.3. Critical heat flux

The knowledge of the values of the critical heat flux \dot{q}_{chf} and critical wall superheat T_{chf} is crucial for predicting chilldown and dryout phenomena in non-equilibriums flows. In nuclear reactor codes. (RELAP5-3D-IV, 2012; TRACE-V5.0, 2007) these values are determined using look-up tables based on extensive experimental measurements obtained under various flow conditions. For cryogenic fluids experimental data remain sparse and values of the \dot{q}_{chf} and T_{chf} are often estimated using mechanistic models (Tong & Tang, 1997; Ghiaasiaan, 2007; Seader et al., 1965; Crowley & Izenson, 1989; Konishi & Mudawar, 2015b). In this work the temperature T_{chf} for the critical heat flux was estimated using approach proposed by Theler (Theler & Freis, 2011) as

$$T_{chf} = \frac{T_s}{1 - \frac{T_s R_g}{h_{lg}} log(2k_g + 1)},$$
(6)

where k_g is the isoentropic expansion factor that for ideal diatomic gases is 7/2 and R_g is the specific gas constant.

In boiling flows the critical heat flux has to be corrected. The corrections have to take into account the dependence of the heat flux on the void fraction, velocity, and sub-cooling of the flow. In this work we used correlations proposed by Griffith et all for cryogenic flows (Franchello, 1993; Seader et al., 1965)

$$\dot{q}_{chf} = \dot{q}_{chf,0}(\alpha_{cr} - \alpha) \left(1 + a_1 \left(\frac{\rho_l c_l \Delta T_{sub}}{\rho_g h_{lg}} \right) (7) + a_2 R e_l + a_3 \left(\frac{R e_l \rho_l c_l \Delta T_{sub}}{\rho_g h_{lg}} \right)^{1/2} \right),$$

where α_{cr} is the critical value of the void fraction and a_i are constants, e.g. $a_1 = 0.0144$, $a_2 = 10^{-6}$, $a_3 = 0.5 \times 10^{-3}$ (Griffith, 1957), and $\alpha_{cr} = 0.96$ (Franchello, 1993) for the water.

The term $\dot{q}_{chf,0}$ in the eq. (7) corresponds to the pool boiling correlations, which were estimated in the present work using Zuber (Zuber & Tribus, 1958) correlations

$$\dot{q}_{chf,0} = \frac{\pi}{24} h_{lg} \rho_g \left(\frac{\sigma g(\rho_l - \rho_g)}{\rho_g^2}\right)^{1/4} \left(\frac{\rho_l}{\rho_l + \rho_g}\right)^{1/2}.$$
 (8)

In numerical tests, we often used a simplified expression for eq. (7), cf (Franchello, 1993; Iloeje, Plummer, Rohsenow, & Griffith, 1982)

$$\dot{q}_{chf} = \dot{q}_{chf,0} \cdot a_1 \cdot (\alpha_{cr} - \alpha)^{a_2} (1 + a_3 G^{a_5}), \qquad (9)$$

where typical values of the parameters used in simulations are $a_1=1.0$, $\alpha_{cr}=0.96$, $a_2=2.0$, $a_3=0.16$, and $a_4=0.2$.

When wall superheat exceeds $\Delta T_{chf} = T_{chf} - T_s$, the transition boiling begins and the heat flux to the wall decreases sharply as a function of the wall temperature until the latter reaches minimum film boiling temperature T_{mfb} .

3.1.4. Minimum film boiling

In the film boiling regime the fluid flow is completely separated from the wall by the vapor film. The minimum value of the wall superheat $\Delta T_{mfb} = T_{mfb} - T_s$ corresponding to this regime was estimated by Berenson as (Carbajo, 1985; Berenson, 1961)

$$\Delta T_{mfb,0} = 0.127 \frac{\rho_g h_{lg}}{\kappa_g} \times \left[\frac{g(\rho_l - \rho_g)}{\rho_l + \rho_g} \right]^{2/3} \left[\frac{\sigma}{g(\rho_l - \rho_g)} \right]^{1/2} \left[\frac{\mu_g}{(\rho_l - \rho_g)} \right]^{1/3}$$
(10)

Iloeje (Franchello, 1993; Iloeje et al., 1982) has corrected Berenson equation to take into account the dependence of the ΔT_{mfb} on the quality and mass flux of the boiling flows in the form

$$\Delta T_{mfb} = c_1 \Delta T_{mfb,0} (1 - c_2 X_e^{c_3}) (1 + c_4 G^{c_5}), \quad (11)$$

where X_e is the equilibrium quality, G is liquid mass flux and a_i are constants, e.g. $a_1 = 0.0144$, $a_2 = 10^{-6}$, $a_3 = 0.5 \times 10^{-3}$ (Griffith, 1957), and $\alpha_{cr} = 0.96$ (Franchello, 1993) for water.

The heat flux in the film boiling flow can be chosen following e.g. recommendations of Groeneveld and Rousseau (Groeneveld & Rousseau, 1983). In this work the heat flux to the wall in the film boiling regime was taken in the form of Bromley correlations

$$h_{br} = C \cdot \left[\frac{g\rho_g \kappa_g^2 \left(\rho_l - \rho_g\right) \tilde{h}_{lg} c_{pg}}{D \left(T_w - T_{spt}\right) P r_g} \right]^{0.25}, \qquad (12)$$

corrected using Iloeje-type correlations (Franchello, 1993; Iloeje et al., 1982)

$$h_{fb} = c_1 h_{br} (1 - c_2 X_e^{c_3}) (1 + c_4 G^{c_5})$$
(13)

Typical values of the parameters used in simulations are the following: (i) $c_1 = 2.0$; (ii) $c_2 = 1.04$; (iii) $c_3 = 2.0$; (iv) $c_4 = 0.2$; (v) $c_5 = 0.1$.

The minimum film boiling heat flux can now be defined as

$$\dot{q}_{mfb} = h_{fb} \Delta T_{mfb}.$$
(14)

To complete the discussion of the boiling heat transfer we notice that in the region of single phase gas flow the heat transfer is given by equations (3) with appropriately modified parameters. Transition to the single phase heat transfer is initiated when dryout transition is detected.

Further details of the constitutive relations, including pressure drop correlations, will be provided elsewhere, see e.g. (D. G. Luchinsky et al., 2016, 2017).

3.2. Uncertainties

Traditionally, the choice of the functional form of the correlations was the major source of uncertainty in cryogenic flow simulations. There have been literally hundreds of various modifications proposed for the flow boiling correlations (Nellis & Klein, 2009; Shahs, 2006) and the corresponding functional space is continuously expanding (S. R. Darr et al., 2015; Kim & Mudawar, 2014; Konishi & Mudawar, 2015a).

In addition, the development of correlations rely on assumptions that can be viewed only as approximations. Furthermore, these approximations usually do not take into account surface wettability, pipe curvature, sub-cooling, and surface orientation.

At the fundamental level the uncertainties in two-fluid modeling stem from the fact that the interface between two phases is continuously fluctuating and neither location nor the shape of the interface can be resolved by the model. The intensity of these fluctuations is especially significant during the chilldown, when liquid and vapor phases coexist under strongly non-equilibrium conditions, see e.g. (Yuan et al., 2007).

Accordingly, the parameters in the correlations discussed above should be considered as unknown fitting parameters of the problem. Their relative importance to the system dynamics is also unknown. And a general probabilistic framework is required to establish statistical distributions of these parameters using available databases of cryogenic flows.

4. INFERENTIAL FRAMEWORK

4.1. Probabilistic approach

The approach to the solution of the inference problem adopted in this work is based on the probabilistic Bayesian method (Ghahramani, 2015). Using this technique one can (Ghahramani, 2015) estimate the conditional probability of unknown model parameters c

$$P(\theta|D,m) = \frac{P(D|c,m)P(\theta|m)}{P(D|m)},$$
(15)

compare different models m

$$P(D|m) = \frac{P(m|D)P(m)}{P(D)}$$
(16)

and forecast system response D_n to untested experimental conditions

$$P(D_n|D,m) = \int P(D_n|\theta, D, m) P(\theta|D, m) d\theta.$$
(17)

In the equations above P(D|c, m) is the likelihood of parameters c in model m. In a typical step of parameter inference within Bayesian probabilistic framework one has to guess or estimate the prior probability P(c|m) and to obtained the improved posterior probability P(c|D, m) of thee model parameters c using available time-series data D.

There are two important advantages of this approach. First is the method's ability to select simpler models over more complex models. Second is the ability to chose a model, which is flexible enough to resolve the complexity of the experimentally observed system dynamics.

4.2. State Space Model

To perform parameter estimation the Eqs. (1) - (2) are integrated over the length of the control volumes (D. G. Luchinsky et al., 2014c; RELAP5-3D-I, 2012). The result of integration at one time step is formally represented in the standard form of the discrete time state space model (SSM)

$$x_{t+1} = f(x_t, c) + \varepsilon_t,$$

$$y_t = g(x_t, b) + \chi_t.$$
(18)

Here x_t is a set of the main dynamical variables of the system $\{\rho_g, \rho_l, T_g, T_l, u_g, u_l, p, \alpha, T_w\}_t^L$ averaged over corresponding control volume at time instant t and c is the set of the model parameters.

The observations y_t in the SSM are related to the unobserved states via nonlinear function $g(x_t, b)$. ε_t and χ_t in equations (18) are independent identically distributed sources of Gaussian noise.

The simultaneous parameter and state estimations in nonlinear system (18) can be performed using a number of techniques, see e.g. (Ghahramani, 2015; Smelyanskiy, Luchinsky, Millonas, & McClintock, 2009; Duggento, Luchinsky, Smelyanskiy, & McClintock, 2009). Here, to simplify the problem we assume that measurement noise can be neglected and that pressure \hat{p} and fluid temperature \hat{T}_f can be measured directly in the experiment.

In the simplest case of general importance the problem is reduced to the curve fitting problem, cf (Cullimore, 1998), which can be solved using global search algorithms availa-



Figure 1. (a) Convergence of the genetic algorithm for simultaneous optimization of 14 model parameters. (b) Best values of the model parameters.

ble in MATLAB optimization toolbox including genetic algorithm, pattern search, simulated annealing, and particle swarm.

An example of convergence is shown in Fig. 1. In this example the genetic algorithm was used for simultaneous optimization over 14 model parameters including characteristic time of the heat transfer to the wall, scaling coefficients for the mass transfer at the interface and at the wetted wall, the film boiling heat transfer, the dependence of the critical heat flux on the void fraction, the heat transfer coefficients on both sides of liquid vapor interface, the heat transfer to the dry wall, the temperatures of the critical heat flux and minimum film boiling, the exponent of the Reynolds number in the Ditus-Boetler correlations at the dry wall, and the parameters of the transition boundary to the dispersed flow regime.

To enforce the convergence an extensive preprocessing was used including sensitivity analysis of the model with respect to the full set of parameters, selection of a subset of the most sensitive parameters for each flow regime, and simplified direct search for initial estimations of sub-optimal values of the selected model parameters. Some further details of the approach can be found in (D. Luchinsky, Khasin, Timucin, Sass, & Brown, 2016).

Below we provide an example of application of this approach to the analysis of chilldown in cryogenic transfer line built at KSC.

5. APPLICATION TO THE ANALYSIS OF THE CRYOGE-NIC LOADING SYSTEM

The time-series data analyzed in this work were obtained at the Simulated Propellant Loading System (SPLS) built at NASA KSC (Johnson, Notardonato, Currin, & Orozco-Smith, 2012).



Figure 2. Sketch of the cryogenic transfer line built at KSC. It includes storage tank (ST) and vehicle tank (VT); the in-line control valves: CV1 through CV8; remotely controlled bleed valves: BV1 through BV8; ten in-line temperature sensors (TT) and 9 in-line pressure sensors (PT).



Figure 3. Model predictions (blue dashed lines) for the fluid temperature are shown in comparison with the experimental time-traces (black lines) at 6 different locations along the transfer line.

5.1. SPLS

The SPLS line includes storage (ST) and vehicle (VT) tanks connected via cryogenic transfer line that has a number of inline (CV) and bleed (BV) valves that control the flow. The flow conditions are monitored using a set of pressure (PT) and temperature (TT) sensors. The sketch of the transfer line indicating the locations of the control valves and sensors is shown in the Fig. 2. The typical childown sequence measured by temperature sensors is illustrated in Fig. 3. The chilldown begins at ~800 sec by opening the valve CV1 (note, that the initial time is chosen arbitrary). At this time all other valves remain closed and after a small temperature drop partial recovery of the temperature measured by sensor TT202 can be observed in Fig. 3(a).

Approximately ~ 270 sec later the valves CV2 and BD 1, 2, and 3 are opened allowing liquid nitrogen to flow down through the system up to the location of the valve CV3. The cooling of the fluid in the pipes can be detected at this stage at temperature sensors TT202 though TT774. The chilldown of the first part of the transfer line is accomplished ~ 1000 sec from the chilldown initiation, when the temperature sensor TT74 indicates the presence of the liquid nitrogen.

The final stage of chilldown begins at \sim 2000 sec, when valve CV3 is opened and nitrogen is allowed to flow through the whole system. The chilldown of the second part of the transfer line can be observed at the sensors TT146 through TT226. The chilldown is completed when sensor TT226 indicates the presence of the liquid nitrogen.

The comparison of the model predictions (green lines in the Fig. 3) with the experimental time traces (black lines) shows that the model can quite accurately reproduce all three stages of the chilldown. We note that the model integration is fast. The integration of nearly 3000 sec of real time shown in the figures takes ~ 10 seconds on a laptop.



Figure 4. The simplified direct search algorithm: convergence of the model predictions (red dashed lines) towards experimental data (solid black lines) for gas temperature measured at four sensors: (a) TT202, (b) TT105, (c) TT162, and (d) TT174. The search is performed for 6 parameters of the SPLS model shown in figure (e). The cost function is shown in figure (f). (top) Initial state with the corresponding initial value of the cost function shown in figure (f). (bottom) Final state.

A good agreement between model predictions and experimental time-series data was achieved using a sequence of steps as will be discussed in more details below.

5.2. Optimization of the SPLS parameters

The optimization of the model parameters involves the following steps: (i) choice of the model parameters; (ii) definition of the objective function; (iii) initial sensitivity study of the parameter's distributions; (iv) estimation of sub-optimal parameter values using simplified direct search; (v) global search for the optimal values of the model parameters; and (vi) estimation of the variance of the optimized parameters.

There are about 98 parameters in the present model of the SPLS. Approximately half of these parameters correspond to the correlation relations. The remaining parameters describe

valve coefficients, minor losses and leaks of the system components. Each parameter is tagged. Any number of parameters can be selected for optimization by listing corresponding tags in an arbitrary order.

We note that in principle the estimation of the model parameters could be facilitated using component based distributed framework. However, a placement of additional sensors along the flow path would be required in this case to monitor the performance of each component. At present such measurements are not available and all the model parameters are estimated simultaneously using time-series data obtained with a few temperature and pressure sensors placed along the line.

The cost function has the form of the sum of square errors on discrete time $t_n = \{t_0, ..., t_N\}$, cf. (Cullimore, 1998)

$$S(\mathbf{c}) = \sum_{n=0}^{N} \sum_{k=1}^{K} \left[\eta_{T_{f}} \left(T_{f,n}^{k}(\mathbf{c}) - \hat{T}_{f,n}^{k} \right)^{2} + \eta_{p} \left(p_{n}^{k}(\mathbf{c}) - \hat{p}_{n}^{k} \right)^{2} \right],$$
(19)

where η_i are weighting coefficients, $T_{f,n}^k(\mathbf{c})$ and $p_{f,n}^k(\mathbf{c})$ are the fluid temperature and pressure predicted by the model at k-th location and n-th instant of time, pressure and temperature with the hat correspond to the measured time-series data, index k runs through different locations of the sensors.

The sensitivity study reveals \sim 30 sensitive model parameters and subsequent optimization was focused on the analysis of this subset of parameters.

The optimization is performed in two steps. At the first step we apply simplified direct search algorithm: (i) the parameter space is discretized on a regular multi-dimensional grid; (ii) parameters are optimized one at a time using 1D search; (iii) the resulting optimal value of a given parameter is used in subsequent searchers; (iv) once the algorithm scans through all the parameters the order of parameters is changed and the search is repeated. It was found that this step is essential to speed up the convergence and to find global minimum.

The convergence of the algorithm is illustrated in the Fig. 4 for simultaneous optimization of 6 parameters, which are scaling factors for the flow coefficients of the valves: Sm151 - input valve CV1; Sc116 - inline valve CV2; Sd120 - dump valve BV3; Sd117 - dump valve BV2; Sd112 - dump valve BV2; and the minimum film boiling heat transfer - qmfbsc.

The obtained sub-optimal values of the model parameters are used as the seed values for the global search. The global optimization was performed using a number of algorithms including genetic algorithm, pattern search, simulated annealing, and particle swarm. An example of convergence of the global search for the optimal values of 14 model parameters using genetic algorithm is shown in Fig. 1.



Figure 5. Comparison of the model predictions for the temperature time-series data (colored dashed lines) with the experimental results (colored solid lines) for the different openings of the valve cv112: (i) 15% blue line; (ii) 25% black line (nominal); (iii) 40% red line.

At the final step we estimate the variance of the optimized model parameters using local search with multiple restarts. This completes the analysis of the updated distributions of the model parameters within general inferential framework.

This procedure can be systematically continued as soon as new experimental data become available. Furthermore, alternative functional forms of the two-phase flow correlations can be compared with each other using proposed framework and available experimental databases.

The proposed approach is flexible and allows one to impose sufficient number of constraints to guarantee physically valid solution of the optimization problem.

To verify the predictions capabilities of the approach we performed the following tests. We modify in the experiment one of the control parameters while keeping all other controls at the fixed values corresponding to the nominal chilldown regime considered in the previous section. To make predictions



Figure 6. Comparison of the model predictions for the pressure time-series data (colored dashed lines) with the experimental results (colored solid lines) for the different openings of the valve cv112: (i) 15% blue line; (ii) 25% black line (nominal); (iii) 40% red line.

we keep the model parameters unchanged except the one modified in the experiment.

The results of model predictions are compared with the experimental time-series in the Figs. 5 and 6. In this particular set of the test measurements the opening of the control valve CV112 (BV1) was 15% (record 0056) and 40% (record 0057) as compared to the nominal opening 25 % (record 0058).

It can be seen from the figures that the results of the model predictions are in good agreement with the pressure timeseries data. The model predictions for the fluid temperature are less accurate, but are still close to the time-traces observed in the experiment.

The results of the model predictions obtained in this work were compared with the results of simulations of the SPLS obtained using commercial software package SINDA/FLUIND (Kashani et al., 2014, 2015) and homogeneous front propagation model (Hafiychuk et al., 2015; Ponizovskaya-Devine et al., 2015b). The present model outperforms both of codes in terms of accuracy, it is also substantially faster than commercial code.

5.3. Application to the fault diagnostics

The proposed algorithm paves the way to the development of the novel physics based approach to the fault diagnostics in the cryogenic flows. The foundation of the novel approach was discussed in our earlier publications (Ponizovskaya-Devine et al., 2015a; Ponizovskaya et al., 2015; Kodali et al., 2015).

In this approach the physics model introduced above is used to build digital fault library and the so called D-matrix (Sheppard & Simpson, 1996) of causal relations between faults and tests (sensor measurements). The D-matrix is used to quickly identify the fault within the ambiguity group and the model based inference can be subsequently applied to disambiguate the fault (Ponizovskaya-Devine et al., 2015a; Ponizovskaya et al., 2015; Kodali et al., 2015). It is known that in general the model-based frameworks can substantially enhance interaction of behavioral knowledge and diagnostic inference (Angeli & Chatzinikolaou, 2004). Our preliminary results confirm this expectation. A more detailed discussion of the development of the on-line expert system for the fault diagnostic of cryogenic transfer will be given elsewhere.

6. CONCLUSIONS

To summarize, we developed an efficient probabilistic framework for simultaneous optimization of a large number of correlation parameters of cryogenic loading system that enables accurate prediction of experimental time-series data. The approach relies on the fast and robust solver for two-fluid cryogenic flow reported in our earlier work. The approach involves the following steps: (i) sensitivity analysis of the model parameters, (ii) simplified direct search for approximate globally optimal values of these parameters, (iii) global stochastic optimization that refines the estimate for parameter values obtained at the previous step, and (iv) estimation of variance of the model parameters using local non-linear optimization.

We validated this approach by analyzing chilldown in the Simulated Propellant Loading System built at NASA KSC. We perform simultaneous optimization of a large number of the model parameters. We demonstrated the convergence of the algorithm towards experimental data using the two main steps of optimization and validate its capability to predict "unseen" experimental time-traces.

We note that the proposed approach paves the way to the development of autonomous control and fault management of cryogenic two-phase flows in the future space missions.

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NOMENCLATURE

- u velocity
- T temperature
- *p* pressure
- e specific energy
- *h* specific enthalpy
- *H* heat transfer coefficient
- g gravity
- Re Reynolds number
- Gr Grashof number
- Pr Prandtl number
- t time
- Δt time step
- A cross-sectional area
- S wall surface area
- V volume of the control volume
- *l* perimeter
- x coordinate along the pipe
- *y* height of the control volume
- \dot{q} heat flux
- c specific heat

Greek

- α gas void fraction
- ρ density
- au wall shear stress
- Γ mass flux per unit volume

Subscript

$egin{array}{c} g \ l \end{array}$	gas liquid
w	wall
i	interface

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BIOGRAPHIES



Dmitry G. Luchinsky is a senior research scientist in MCT Inc. He obtained his MSc and PhD in physics in Moscow working on nonlinear optics of semiconductors. He is an author of more than 100 publications. He has been on a number of occasions a Royal Society Visiting Fellow and a NASA visiting scientist. He worked as a senior scien-

tific researcher in VNII for Metrological Service (Moscow, Russia) and as a Senior Research Fellow in Lancaster University (Lancaster, UK). His research interests include nonlinear optics, stochastic and chaotic nonlinear dynamics, dynamical inference, fluid dynamics, ionic motion. His research is currently focused on theory and CFD of gas dynamics and cryogenic flows.



Michael Khasin Dr Michael Khasin is a Senior Researcher in SGT Inc., working at NASA Ames Research Center. He holds B.Sc. in Physics (Honors Program), 2001, M.Sc. in physics, 2003, and PhD in chemical physics, 2008, from the Hebrew University of Jerusalem. As a postdoctoral researcher at Michigan State University, Mas-

sachusetts Institute of Technology, and University of Michi-

gan, Michael worked on the theory of non-equilibrium systems and their control and transport in disordered system. His research interests include applied physics, nonlinear and stochastic dynamics, large fluctuations and their control in non-equilibrium systems and efficient simulation of complex dynamics. He has been an invited speaker to many international and national conferences and workshops. Currently his research is focused on the theory of heat transfer, fluid dynamics, and fluid structure interaction.



Dŏgan A. Timuçin eccived the B.S. degree from Middle East Technical University, Ankara, Turkey, in 1989, and the M.S. and Ph.D. degrees from Texas Tech University, Lubbock, TX, USA, in 1991 and 1994, respectively, all in electrical engineering. He has been with the National Aeronautics and Space Administration Ames Research Cen-

ter, Mountain View, CA, USA, since 1995. He has been involved in research on holographic optical memories, quantum computing algorithms, and radiative transfer models for remote sensing, statistical physics models for air traffic control, and most recently, modeling and inference of faults in electrical wiring and interconnect systems. His current research interests include selective laser melting of metal powders and nondestructive inspection of composite structures.