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# A homogeneous non-equilibrium two-phase critical flow model

J.R. Travis<sup>a</sup>, D. Piccioni Koch<sup>b,\*</sup>, W. Breitung<sup>c</sup>

<sup>a</sup> Engineering & Scientific Software, Inc., 2128 S. Ensenada Circle, Rio Rancho, NM 87124, USA

<sup>b</sup> Steinbuch Centre for Computing (SCC), Karlsruher Institut für Technologie (KIT), Postfach 3640, 76021 Karlsruhe, Germany

<sup>c</sup> simaps GmbH, Rietburgweg 5, 76751 Jockgrim, Germany

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## ABSTRACT

A non-equilibrium two-phase single-component critical (choked) flow model for cryogenic fluids is developed from first principle thermodynamics. Modern equations-of-state (EOS) based upon the Helmholtz free energy concepts are incorporated into the methodology. Extensive validation of the model is provided with the NASA cryogenic data tabulated for hydrogen, methane, nitrogen, and oxygen critical flow experiments performed with four different nozzles. The model is used to develop a hydrogen critical flow map for stagnation states in the liquid and supercritical regions.

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## 1. Introduction

The work described in the present paper was initiated in the frame of the *icefuel*<sup>®</sup> (Integrated Cable Energy system for FUEL and power) project [1], which aimed to create an Infrastructure System for Cryogenic Hydrogen Storage, Distribution and Decentral Reconversion.

The concept is based on the production and liquefaction of hydrogen to buffer large quantities of excess renewable electricity, mainly produced in facilities such as wind and solar power plants. A schematic view of the *icefuel*<sup>®</sup> system is shown in Fig. 1. The cryogenic hydrogen (<40 K) involved in this project was distributed through a grid of superinsulated pipes. Safety related consequences of cryogenic hydrogen releases from *icefuel*<sup>®</sup> cables were investigated both theoretically and experimentally at the Institute for Nuclear and Energy Technology (IKET) of the Karlsruhe Institute of Technology (KIT) (Germany). In order to investigate the safety

consequences of small leaks or holes in the cables and estimate consequent discharges, dedicated simulation codes were developed and applied.

In this paper, the development of a homogeneous, non-equilibrium, two-phase, critical flow model for cryogenic fluids based upon first principal thermodynamics is described. The model can be used to accurately calculate discharge mass flow rates from high pressure reservoirs.

## 2. Critical flow and two-phase critical flow models

The critical flow, also referred to as choking or choked flow, is defined in terms of Mach number,  $M = U/c$ , where  $U$  is the fluid flow speed and  $c$  is the speed of sound. For critical flows, the Mach number is unitary, increases for supersonic flows ( $M > 1$ ) and decreases for subcritical ones ( $M < 1$ ).

\* Corresponding author.

E-mail addresses: [jack\\_travis@comcast.net](mailto:jack_travis@comcast.net) (J.R. Travis), [daniela.piccioni@kit.edu](mailto:daniela.piccioni@kit.edu) (D. Piccioni Koch), [breitung@simaps.de](mailto:breitung@simaps.de) (W. Breitung).

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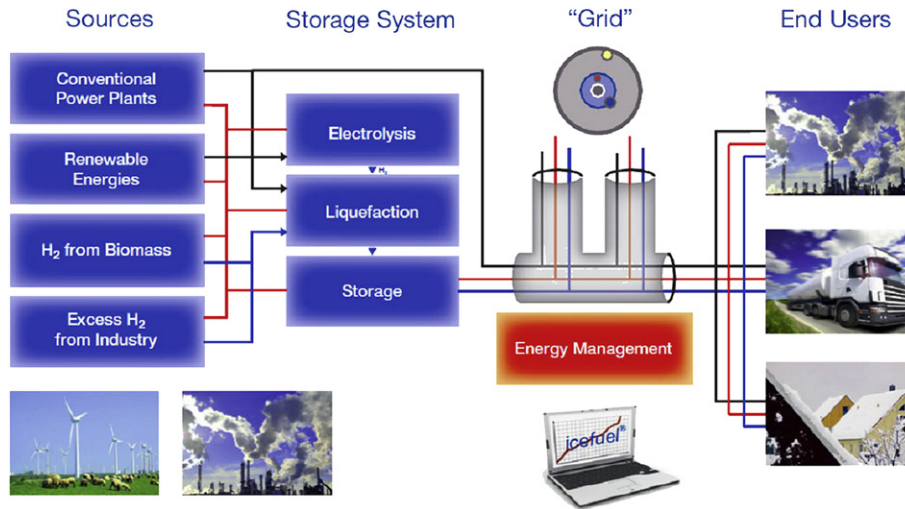


Fig. 1 – icefuel® schematic [1].

Starting from 1947 with the work of J.G. Burnell [2] many theories have been developed for the calculation of the two-phase critical flow and several classification criteria have been used to order such theories. A first classification distinguishes between homogeneous and non-homogeneous models. Homogeneous models assume that the liquid and vapor are mixed together and can be treated as a mixture, while in the non-homogeneous models, the liquid and vapor exist as separated phases. Another relevant criterion of classification is the thermodynamic equilibrium. Some models assume Thermodynamic Equilibrium, i.e. both phases coexist at the same saturation conditions (Thermal Equilibrium), are well-mixed, with equal velocity (Dynamic Equilibrium) and with phase densities constant during expansion (Chemical Equilibrium); the non-equilibrium models assume no thermodynamic equilibrium. Some relevant two-phase critical flow models are reviewed in [3–5] and are not further discussed in this paper. Hereafter, the development of our homogeneous, non-equilibrium two-phase critical flow model is described.

### 3. Modern equations of state

Modern equations-of-state [6] are often formulated using the Helmholtz energy as the fundamental property with independent variables of temperature and density,

$$\alpha(T, \rho) = \alpha^0(T, \rho) + \alpha^r(T, \rho), \tag{1}$$

where  $\alpha$  is the Helmholtz energy,  $\alpha^0(T, \rho)$  is the ideal gas contribution to the Helmholtz energy, and  $\alpha^r(T, \rho)$  is the residual Helmholtz energy, which corresponds to the influence of intermolecular forces in real gases. Thermodynamics properties can be calculated as derivatives of the Helmholtz energy. For example, the pressure can be expressed as

$$p = \rho^2 \left( \frac{\partial \alpha}{\partial \rho} \right)_T. \tag{2}$$

In practical applications, the functional form is explicit in the dimensionless Helmholtz energy,  $\alpha$ , using independent variables of dimensionless density and temperature. The form of this equation is

$$\frac{\alpha(T, \rho)}{RT} = \alpha(\tau, \delta) = \alpha^0(\tau, \delta) + \alpha^r(\tau, \delta) \tag{3}$$

where  $\tau = T_c/T$ , the inverse reduced temperature,  $\delta = \rho/\rho_c$ , the reduced density and  $R$  is the universal gas constant (8.314510 J/(mol K)).

The ideal gas Helmholtz energy is often represented in the computational convenient parameterized form

$$\alpha^0(\tau, \delta) = \ln \delta + a_0 \ln \tau + a_1 + a_2 \tau + \sum_{k=3}^N a_k \ln[1 - \exp(b_k \tau)], \tag{4}$$

and the residual contribution to the Helmholtz free energy takes the form

$$\alpha^r(\tau, \delta) = \sum_{i=1}^l N_i \delta^{d_i} \tau^{t_i} + \sum_{i=1}^m N_i \delta^{d_i} \tau^{t_i} \exp(-\delta^{p_i}) + \sum_{i=m+1}^n N_i \delta^{d_i} \tau^{t_i} \exp \left[ \varphi_i (\delta - D_i)^2 + \beta_i (\tau - \gamma_i)^2 \right], \tag{5}$$

where the parameters and coefficients in these expressions are given for hydrogen (normal, parahydrogen and orthohydrogen) [7], oxygen [8], nitrogen [9], methane [10], and water [11].

The advantages of this explicit formulation in the Helmholtz free energy become apparent for the calculation of enthalpy, entropy, and sound speed, respectively:

$$h(T, \rho) = RT \left\{ \tau \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_\delta + \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right] + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + 1 \right\}, \tag{6}$$

$$s(T, \rho) = R \left\{ \tau \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_\delta + \left( \frac{\partial \alpha^r}{\partial \tau} \right)_\delta \right] - \alpha^0 - \alpha^r \right\}, \text{ and} \tag{7}$$

$$w(T, \rho) = \sqrt{\frac{RT}{M} \left[ 1 + 2\delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau + \delta^2 \left( \frac{\partial^2 \alpha^r}{\partial \delta^2} \right)_\tau - \frac{\left[ 1 + \delta \left( \frac{\partial \alpha^r}{\partial \delta} \right)_\tau - \delta \tau \left( \frac{\partial^2 \alpha^r}{\partial \delta \partial \tau} \right) \right]^2}{\tau^2 \left[ \left( \frac{\partial^2 \alpha^0}{\partial \tau^2} \right)_\delta + \left( \frac{\partial^2 \alpha^r}{\partial \tau^2} \right)_\delta \right]} \right]}. \tag{8}$$

Other fluid properties can be found in references [6,12].

The saturation line can be described by the ancillary equation [6] for the saturated vapor-pressure,  $p_{\text{sat}}$  as

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