ON SOLUTIONS TO EQUILIBRIUM PROBLEMS FOR SYSTEMS OF STIFFENED GASES[*]

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Abstract. We consider an isolated system of N immiscible fluids, each following a stiffened-gas equation of state. We consider the problem of calculating equilibrium states from the conserved fluid-mechanical properties, i.e., the partial densities and internal energies. We consider two cases; in each case mechanical equilibrium is assumed, but the fluids may or may not be in thermal equilibrium. For both cases, we address the issues of existence, uniqueness, and physical validity of equilibrium solutions. We derive necessary and sufficient conditions for physically valid solutions to exist, and prove that such solutions are unique. We show that for both cases, physically valid solutions can be expressed as the root of a monotonic function in one variable. We then formulate efficient algorithms which unconditionally guarantee global and quadratic convergence toward the physically valid solution.

1. Introduction. Due to its simplicity and suitability for fluid-mechanical applications, the stiffened-gas equation of state advocated by Menikoff [7] and Menikoff and Plohr [8] has found widespread use in the computational fluid dynamics community [4, 6, 17]. In particular, many authors consider it a useful basis for simulating multicomponent flow problems [1, 3, 11, 12, 14, 16]. This observation motivates our current work.

For a given fluid, the stiffened-gas equation of state can be written as a pressure law:

$$(1) \qquad p(\rho, e) = (\gamma - 1)\rho(e - e_*) - \gamma p_\infty,$$

where p is the pressure, ρ is the density, and e is the specific internal energy of the fluid. The parameters γ, e_*, and p_∞ are constants specific to the fluid. Herein, e_* defines the zero point for the internal energy and becomes relevant when phase transitions are involved. The parameter p_∞ leads to the "stiffened" properties compared to ideal gases; a large value of p_∞ implies near-incompressible behavior. Note in particular that for $p_\infty = 0$ an ideal-gas law is recovered.

In this paper, we consider N immiscible fluids, each governed by the stiffened-gas law (1) while sharing a common volume V. Now let M_i be the total mass of fluid i

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in the volume V. We may then define *partial densities* m_i as

$$(2) \qquad m_i = \frac{M_i}{V}.$$

Furthermore, let V_i be the total volume occupied by the fluid i, defined by

$$(3) \qquad V_i = \frac{M_i}{\rho_i},$$

where ρ_i is the density of fluid i. We may then define the *volume fractions* α_i as

$$(4) \qquad \alpha_i = \frac{V_i}{V},$$

where consistency requires that

$$(5) \qquad \sum_{i=1}^{N} \alpha_i = 1.$$

From (2)–(4) it now follows that the partial densities can be written as

$$(6) \qquad m_i = \rho_i \alpha_i.$$

Furthermore, each fluid has a partial internal energy density E_i given by

$$(7) \qquad E_i = m_i e_i,$$

and the total internal energy density in the volume V is

$$(8) \qquad E = \sum_{i=1}^{N} E_i.$$

Fluid-mechanical models are typically expressed as partial differential equations representing conservation or balance laws. The solution vector obtained from these equations will typically provide us with the partial densities (6) and energies (7) or (8). From this information, our task is to calculate the proper physical equilibrium states.

In this paper, we will consider two cases, summarized as follows.

PROBLEM 1. *The partial densities* (6) *are known for each of the N fluids. The internal energies* (7) *are also known for each of the N fluids. In addition, we assume that the fluids are in mechanical equilibrium; they all have the same pressure. Our task is to calculate the pressure p and the temperatures T_i for each fluid as well as the volume fractions α_i.*

This problem is more precisely defined in section 3.

PROBLEM 2. *The partial densities* (6) *are known for each of the N fluids. The total internal energy* (8) *is known for the mixture. In addition, we assume that the fluids are in mechanical* and *thermal equilibrium; they all have the same pressure and temperature. Our task is to calculate the pressure p, the common temperature T, as well as the volume fractions α_i.*

This problem is more precisely defined in section 4.

These problems have been encountered and solved by many authors [2, 3, 9, 10, 13, 15], although the number of fluids has often been limited to $N = 2$. Our current paper is motivated by the observation that a complete discussion of the question of

existence, uniqueness, and physical validity of solutions to such general equilibrium problems for N fluids seems so far to be lacking in the literature.

A main result of this paper is a proof that, for any system of stiffened gases, if physically valid (in a sense that will be made precise) solutions to the equilibrium Problems 1 and 2 exist, they are unique. This should not be surprising; in many cases, existence and uniqueness can be established directly by thermodynamic stability theory if the equilibrium solution corresponds to the minimum of some free energy for the system. One may then apply convexity arguments as described, for instance, in [5].

However, in this paper we are also interested in obtaining *explicit* conditions for physically valid solutions to exist, as well as practical algorithms for obtaining these solutions. Toward this aim, a simple constructive approach will turn out to be fruitful. A main idea behind our approach is the observation that, although the problems are highly nonlinear, the stiffened-gas equation of state is in itself sufficiently linear to allow the volume fractions to be expressed without an explicit temperature dependence. This has been done in (42) and (79); see below.

This strategy allows for reducing Problems 1 and 2 to finding the root of a monotonic function in one variable, for which existence and uniqueness follow directly from elementary arguments. Robust and efficient numerical solvers can also be rather straightforwardly constructed.

Our paper is organized as follows. In section 2, we review the stiffened-gas equation of state as presented by Menikoff and Plohr [7, 8]. In section 3, we address equilibrium Problem 1; here equal pressures are assumed, but the fluids have independent temperatures. A key equation is (42), which allows us to directly construct a monotonic function whose root is our required solution.

In section 4 we address the case where both mechanical and thermal equilibrium are assumed; this is Problem 2 described above. Here we use (79) for the construction of our monotonic function, which in this case requires an additional mathematical transformation detailed in section 4.1.1. For both problems, we derive sufficient and necessary conditions for physically valid solutions to exist, and uniqueness follows from monotonicity.

In section 5, we take advantage of some well-established properties of the Newton–Raphson method. In particular, we show how our problems may be formulated to yield numerical solution algorithms which unconditionally guarantee global and quadratic convergence.

In section 6, we present numerical examples to verify and illustrate the results derived in section 5. Finally, we briefly summarize our results in section 7.

2. The stiffened-gas equation of state. In this section, we briefly review some properties of the *stiffened-gas* equation of state considered in this paper. We refer to the work of Menikoff and Plohr [8] for a more in-depth discussion, particularly regarding the physical basis for this model.

For a given fluid, the stiffened-gas equation of state is fully defined by the *Helmholtz free energy* [7]:

$$(9) \qquad A(\rho, T) = c_V T \left(1 - \ln \left(\frac{T}{T_0} \right) + (\gamma - 1) \ln \left(\frac{\rho}{\rho_0} \right) \right) - s_0 T + \frac{p_\infty}{\rho} + e_*,$$

where the parameters c_V, γ, p_∞, T_0, ρ_0, s_0, and e_* are constants specific to the fluid. Here e_* is used to define the zero point of energy, which becomes relevant when phase transitions are involved. Although phase transitions will not be considered in this

paper, we include this parameter for completeness.

2.1. Entropy. From (9) we can derive the entropy

$$(10) \qquad s(\rho, T) = -\left(\frac{\partial A}{\partial T}\right)_\rho = c_V \ln\left(\frac{T}{T_0}\left(\frac{\rho_0}{\rho}\right)^{\gamma-1}\right) + s_0.$$

Note that

$$(11) \qquad s_0 = s(\rho_0, T_0).$$

Hence the stiffened-gas equation of state can be interpreted as a *local linearization* near the state (ρ_0, T_0), where the entropy is s_0.

2.2. Heat capacity. The intensive internal energy is given by

$$(12) \qquad e(\rho, T) = A + Ts = c_V T + \frac{p_\infty}{\rho} + e_*,$$

from which we immediately see that c_V is the *specific isochoric heat capacity*:

$$(13) \qquad c_V = \left(\frac{\partial e}{\partial T}\right)_\rho.$$

2.3. Pressure. The pressure is obtained by

$$(14) \qquad p(\rho, T) = \rho^2\left(\frac{\partial A}{\partial \rho}\right)_T = \rho(\gamma-1)c_V T - p_\infty.$$

By (12), this can be written as the pressure law (1):

$$(15) \qquad p(\rho, e) = (\gamma-1)\rho(e - e_*) - \gamma p_\infty,$$

and we also obtain the energy in terms of pressure and temperature:

$$(16) \qquad e(p, T) = c_V T \frac{p + \gamma p_\infty}{p + p_\infty} + e_*.$$

Note that positive densities and energies do not generally guarantee positivity of the pressure.

2.4. Ratio of specific heats. Substituting (14) into (10), we obtain

$$(17) \qquad s(p, T) = \gamma c_V \ln\left(\frac{T}{T_0}\left(\frac{p_0 + p_\infty}{p + p_\infty}\right)^{1-1/\gamma}\right) + s_0,$$

where

$$(18) \qquad p_0 = p(\rho_0, T_0).$$

Now

$$(19) \qquad c_p = T\left(\frac{\partial s}{\partial T}\right)_p = \gamma c_V;$$

hence γ is the *ratio of specific heats*

$$(20) \qquad \gamma = \frac{c_p}{c_V},$$

and it follows that c_p is constant.

2.5. Sound velocity. Now if we introduce the constant

$$
(21) \qquad K = \frac{e^{s_0/c_p}}{T_0} \left(p_0 + p_\infty\right)^{1-1/\gamma},
$$

we can write (17) more conveniently as

$$
(22) \qquad s(p, T) = c_p \ln\left(KT \left(p + p_\infty\right)^{1/\gamma - 1}\right).
$$

Then from (14) we get the relation

$$
(23) \qquad s(p, \rho) = c_p \ln\left(K \frac{\left(p + p_\infty\right)^{1/\gamma}}{\rho(\gamma - 1)c_V}\right).
$$

Hence

$$
(24) \qquad \mathrm{d}s = \frac{c_p}{\gamma(p + p_\infty)}\,\mathrm{d}p - \frac{c_p}{\rho}\,\mathrm{d}\rho
$$

and

$$
(25) \qquad c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \gamma \frac{p + p_\infty}{\rho}.
$$

Hence p_∞ can be interpreted as a parameter that "stiffens" an ideal gas by increasing its sound velocity.

We further note that from (12) and (14) we get a simple expression for the specific enthalpy:

$$
(26) \qquad h = e + \frac{p}{\rho} = c_p T + e_*.
$$

From this and (15), expression (25) can be written as

$$
(27) \qquad c^2 = (\gamma - 1)c_p T.
$$

2.6. Physical considerations. We note that the various parameters of the stiffened-gas equation of state cannot be chosen freely if physically correct thermodynamic behavior is to be reproduced. Throughout this paper, we will consistently make the assumption that the parameters satisfy the following standard restrictions, which follow from thermodynamic stability theory.

RESTRICTION 1. *We require*

$$
(28) \qquad c_V > 0
$$

and

$$
(29) \qquad \gamma > 1
$$

for the stiffened-gas equation of state to be physically valid.

3. Mechanical equilibrium. In this section, we consider a mixture of N fluids, each following its separate stiffened-gas equation of state (9). We assume that the fluids are immiscible, in the sense that the equation of state is not affected by the mixing. We here assume that the fluids reach instantaneous mechanical equilibrium, but heat transfer is dynamically modelled. Hence the fluids possess individual temperatures.

For each fluid $i \in \{1, \ldots, N\}$, the following information is known to us:
- The partial densities $m_i = \rho_i \alpha_i$.
- The internal energies $E_i = m_i e_i$.

Herein, the densities are given by (14),

$$(30) \qquad \rho_i = \frac{p + p_{\infty,i}}{(\gamma_i - 1)c_{V,i}T_i} \quad \forall i,$$

the volume fractions are given by (4), and the internal energies are given by (12),

$$(31) \qquad e_i = c_{V,i}T_i + \frac{p_{\infty,i}}{\rho_i} + e_{*,i}.$$

DEFINITION 1 (Problem 1). *Given the information above, our task is to calculate the common pressure p, the temperatures T_i, and the volume fractions α_i.*

Such a problem is considered, for instance, in [3, 10, 13]. We now define the following classes of solutions.

DEFINITION 2. *A* valid *solution to Problem* 1 *is a solution that satisfies*

$$(32) \qquad \alpha_i \in (0,1] \quad \forall i$$

and

$$(33) \qquad \sum_{i=1}^{N} \alpha_i = 1.$$

A physically valid *solution to Problem* 1 *is a valid solution that satisfies*

$$(34) \qquad 0 < \rho_i < \infty,$$
$$(35) \qquad 0 < T_i < \infty,$$
$$(36) \qquad e_{*,i} < e_i < \infty$$

for all i.

A strictly valid *solution to Problem* 1 *is a physically valid solution that satisfies*

$$(37) \qquad p > 0.$$

Note that, by Definition 2, nonpositive partial densities (6) cannot yield physically valid solutions. Hence we have the following.

RESTRICTION 2. *Physically valid solutions require*

$$(38) \qquad m_i > 0 \quad \forall i.$$

With (36), this immediately yields the following additional restriction.

RESTRICTION 3. *Physically valid solutions require*

$$(39) \qquad E_i - m_i e_{*,i} = m_i(e_i - e_{*,i}) > 0 \quad \forall i.$$

Furthermore, we make the following observation.

LEMMA 1. *Any physically valid solution must satisfy*

$$(40) \qquad p \in \mathcal{P}_1, \quad where \quad \mathcal{P}_1 = \left(-\min_i p_{\infty,i}, +\infty \right).$$

Proof. The lemma follows directly from Restriction 1 and from (34) applied to (30). □

REMARK 1. *Note that if*

$$(41) \qquad \min_i p_{\infty,i} \geq 0,$$

then it follows from Restriction 1, Lemma 1, and (16) that the condition (36) is superfluous; it follows directly from (34).

3.1. Mathematical formulation of the problem. Multiplying (15) with α_i and using (6)–(7), we obtain

$$(42) \qquad \alpha_i = \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{p + \gamma_i p_{\infty,i}},$$

from which we immediately obtain the following.

LEMMA 2. *Any physically valid solution must satisfy*

$$(43) \qquad p \in \left(-\min_i (\gamma_i p_{\infty,i}), +\infty \right).$$

Proof. In order for (32) to be satisfied by (42), it follows from Restrictions 1 and 3 that we must have

$$(44) \qquad p + \gamma_i p_{\infty,i} > 0 \qquad \forall i,$$

which is equivalent to (43). □

An equation for the pressure is now found by imposing the condition that the volume fractions (42) must sum to 1. In other words, if we consider the function

$$(45) \qquad f(\hat{p}) = \sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{\hat{p} + \gamma_i p_{\infty,i}},$$

the required pressure p must satisfy

$$(46) \qquad f(p) = 1.$$

LEMMA 3. *The equation*

$$(47) \qquad f(\hat{p}) = 1$$

has a unique solution for $\hat{p}$ satisfying

$$(48) \qquad \hat{p} \in \mathcal{P}_2, \quad where \quad \mathcal{P}_2 = \left(-\min_i (\gamma_i p_{\infty,i}), +\infty \right).$$

Proof. We note that $f(\hat{p})$ is a rational function without poles in the interval $\mathcal{P}_2$. Hence $f(\hat{p})$ is C^∞-smooth in this interval, and its first derivative is

$$(49) \qquad \frac{\mathrm{d}f}{\mathrm{d}\hat{p}} = -\sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{\left(\hat{p} + \gamma_i p_{\infty,i} \right)^2}.$$

From (29) and Restriction 3 it follows that $f'(\hat{p}) < 0$ throughout the interval $\mathcal{P}_2$. Furthermore, note that $f(\hat{p}) \to +\infty$ as $\hat{p} \to -\min_i (\gamma_i p_{\infty,i})^+$. Also,

$$\lim_{\hat{p} \to +\infty} f(\hat{p}) = 0. \tag{50}$$

Uniqueness and existence of the solution to (47) in the interval $\mathcal{P}_2$ follow. $\square$

We now know that $f(\hat{p}) = 1$ has a unique solution in the interval $\mathcal{P}_2$. However, Lemma 1 tells us that the solution must also lie in the interval $\mathcal{P}_1$ for the solution to be physically valid. This is trivially satisfied if

$$\min_i p_{\infty,i} \leq 0. \tag{51}$$

Otherwise, we observe that $f(\hat{p})$ is monotonically decreasing in the interval $\mathcal{P}_1$. We must then have

$$\lim_{\hat{p} \to -\min_i p_{\infty,i}^+} f(\hat{p}) > 1 \tag{52}$$

for a physically valid solution to exist. Together with (45), this yields the following restriction.

RESTRICTION 4. *Physically valid solutions require either*

$$\min_i p_{\infty,i} \leq 0 \tag{53}$$

or

$$\sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{\gamma_i p_{\infty,i} - \min_j p_{\infty,j}} > 1. \tag{54}$$

To recapitulate, we have the following claim.

LEMMA 4. *If Problem* 1 *has a physically valid solution in the sense of Definition* 2, *then E_i and m_i satisfy Restrictions* 2–4.

Proof. From (6), (32), and (34) it follows that Restriction 2 is satisfied. Restriction 3 follows from (36) and Restriction 2. By Lemmas 1 and 2, it follows from the monotonicity of f that Restriction 4 is satisfied. $\square$

Furthermore, the converse also holds, as given next.

LEMMA 5. *Problem* 1 *has a physically valid solution in the sense of Definition* 2 *if E_i and m_i satisfy Restrictions* 2–4.

Proof. Lemma 3 guarantees the existence of a solution satisfying (33). Furthermore, from (42), Lemma 2, and Restrictions 1 and 3 it follows that (32) is satisfied. Hence the solution is valid.

Given that (32) is satisfied, it follows from Restriction 2 and (6) that (34) is satisfied. Furthermore, Restriction 4 guarantees that (40) is satisfied. Given that (34) is satisfied, it now follows from (30) that (35) is satisfied. Finally, from (16), Restriction 1, and Lemmas 1–2 it follows that (36) is satisfied. Hence the solution is physically valid. $\square$

We are now in position to conclude the following.

PROPOSITION 1. *Problem* 1 *has a physically valid solution in the sense of Definition* 2 *if and only if E_i and m_i satisfy Restrictions* 2–4. *This solution is unique.*

Proof. By Lemmas 4 and 5, all that remains is to prove uniqueness. Uniqueness of the pressure follows directly from Lemma 3. Then the volume fractions are uniquely determined by (42). Multiply (31) by m_i to obtain

$$E_i = m_i c_{V,i} T_i + \alpha_i p_{\infty,i} + m_i e_{*,i}, \tag{55}$$

and it follows that T_i is uniquely determined for all i. $\square$

3.2. Positivity of the pressure. We note that Definition 2 of physically valid solutions allows for negative pressures. This is consistent with the view that a *stiffened* gas is obtained by shifting the zero point of pressure for an *ideal* gas. In particular, all derived thermodynamic quantities are well defined as long as $p + p_{\infty,i}$ remains positive; see, for instance, (17) and (30).

Hence there is no immediate reason to discard negative-pressure solutions as unphysical. However, one may easily envisage situations in which positivity of the pressure must be enforced, for instance if the stiffened gas mixture is to be used in conjunction with other models. We now observe the following.

RESTRICTION 5. *A physically valid solution to Problem 1 is a strictly valid solution in the sense of Definition 2 if and only if one of the following requirements is satisfied: either*

$$(56) \qquad \min_i p_{\infty,i} \leq 0$$

or

$$(57) \qquad \sum_{i=1}^{N} \frac{E_i - m_i e_{*,i}}{p_{\infty,i}} \frac{\gamma_i - 1}{\gamma_i} > 1.$$

Proof. If (56) holds, it follows from Lemma 1 that any physically valid solution is also a strictly valid solution. Otherwise, since $f(\hat{p})$ as given by (45) is a strictly decreasing function for $\hat{p} > 0$, it follows that a positive solution to (47) requires

$$(58) \qquad f(0) > 1.$$

This is precisely the condition (57). Conversely, if the solution satisfies $p \leq 0$, then $f(0) \leq 1$. □

Furthermore, we may make a more precise statement, as follows.

PROPOSITION 2. *Problem 1 has a strictly valid solution in the sense of Definition 2 if and only if E_i and m_i satisfy Restrictions 2–3 as well as Restriction 5. This solution is unique.*

Proof. Note that by (29) and Restriction 3, the following inequality holds whenever $\min_i p_{\infty,i} > 0$:

$$(59) \qquad \sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{\gamma_i p_{\infty,i} - \min_j p_{\infty,j}} > \sum_{i=1}^{N} \frac{E_i - m_i e_{*,i}}{p_{\infty,i}} \frac{\gamma_i - 1}{\gamma_i}.$$

Hence Restriction 5 implies Restriction 4. The result now follows from Proposition 1 and Restriction 5. □

4. Thermal and mechanical equilibrium. In this section, we consider a modified problem where the additional assumption is made that the fluids are in thermal equilibrium. We again consider a mixture of N immiscible fluids, each following its separate stiffened-gas equation of state (9).

For each fluid $i \in \{1, \ldots, N\}$, the following information is known to us:
- The partial densities $m_i = \rho_i \alpha_i$.
- The total energy density of the mixture $E = \sum_{i=1}^{N} m_i e_i$.

Herein, the densities are given by (14),

$$(60) \qquad \rho_i = \frac{p + p_{\infty,i}}{(\gamma_i - 1)c_{V,i}T} \quad \forall i,$$

and the internal energies are given by (12),

$$e_i = c_{V,i}T + \frac{p_{\infty,i}}{\rho_i} + e_{*,i}. \tag{61}$$

DEFINITION 3 (Problem 2). *Given the information above, our task is to calculate the common pressure p, the common temperature T, and the volume fractions α_i.*

This problem is considered in [2, 9]. Analogously to section 3, we define a hierarchy of classes of solutions below.

DEFINITION 4. *A* valid *solution to Problem 2 is a solution that satisfies*

$$\alpha_i \in (0,1] \quad \forall i \tag{62}$$

and

$$\sum_{i=1}^{N} \alpha_i = 1. \tag{63}$$

A physically valid *solution to Problem 2 is a valid solution that satisfies*

$$0 < \rho_i < \infty \quad \forall i, \tag{64}$$
$$0 < T < \infty. \tag{65}$$

A positive-energy *solution to Problem 2 is a physically valid solution that satisfies*

$$e_{*,i} < e_i < \infty \quad \forall i. \tag{66}$$

A strictly valid *solution to Problem 2 is a physically valid solution that satisfies*

$$p > 0. \tag{67}$$

REMARK 2. *Compared to Problem 1, here we have chosen to split physically valid solutions into two classes, where positive energies may or may not be imposed. This is done with the aim of completeness, as the separate analysis of these two cases allows for the option of relaxing the requirement* (66).

As in section 3, the following restriction follows from (6).

RESTRICTION 6. *Physically valid solutions require*

$$m_i > 0 \quad \forall i. \tag{68}$$

REMARK 3. *Note that in the limit when a component vanishes, i.e.,*

$$\exists j \in \{1,\ldots,N\} : m_j = 0, \tag{69}$$

our analysis can still be applied with a minor modification. Assume that K of the N components satisfy

$$m_j = 0 \quad \forall j \in \{1,\ldots,K\}, \tag{70}$$

where $K < N$. It then follows from (6) *and* (64) *that*

$$\alpha_j = 0 \quad \forall j \in \{1,\ldots,K\}. \tag{71}$$

We may then replace the problem with an equivalent problem consisting of $M = N - K$ components, where the volume fractions satisfy

$$\alpha_r \in (0, 1] \quad \forall r \in \{K + 1, \dots, N\} \tag{72}$$

and

$$\sum_{r=K+1}^{N} \alpha_r = 1. \tag{73}$$

We may now apply our results to this reduced problem. This consideration is equally valid for Problem 1, with the understanding that the temperatures T_j would then be undefined for the vanishing components.

Furthermore, as it did for Problem 1, the following result holds.

LEMMA 6. *Any physically valid solution must satisfy*

$$p \in \mathcal{P}_1, \quad where \quad \mathcal{P}_1 = \left(-\min_i p_{\infty,i}, +\infty\right). \tag{74}$$

Proof. The lemma follows directly from Restriction 1 and Definition 4 applied to (60). $\quad\square$

4.1. Mathematical formulation of the problem. Multiplying (26) with m_i, we obtain

$$\alpha_i \left(\rho_i(e_i - e_{*,i}) + p\right) = m_i c_{p,i} T. \tag{75}$$

Also, (15) can be written as

$$\rho_i(e_i - e_{*,i}) + p = \frac{\gamma_i}{\gamma_i - 1} \left(p + p_{\infty,i}\right); \tag{76}$$

hence

$$\alpha_i \frac{\gamma_i}{\gamma_i - 1} \left(p + p_{\infty,i}\right) = m_i c_{p,i} T. \tag{77}$$

Furthermore, summing (75) over all i yields

$$E + p - \sum_{i=1}^{N} m_i e_{*,i} = T \sum_{i=1}^{N} m_i c_{p,i}. \tag{78}$$

Substituting for T in (77), we obtain

$$\alpha_i = \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{\sum_{j=1}^{N} m_j c_{p,j}} \frac{E + p - \sum_{j=1}^{N} m_j e_{*,j}}{p + p_{\infty,i}}. \tag{79}$$

As in section 3, an equation for the pressure is found by imposing the condition that the volume fractions (79) must sum to 1. We introduce the function

$$g(\hat{p}) = \sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{\sum_{j=1}^{N} m_j c_{p,j}} \frac{E + \hat{p} - \sum_{j=1}^{N} m_j e_{*,j}}{\hat{p} + p_{\infty,i}}, \tag{80}$$

where the required pressure p must satisfy

$$g(p) = 1. \tag{81}$$

4.1.1. A simplifying notation. Now note that if we introduce the variables

$$(82) \qquad A_i = \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{\sum_{j=1}^{N} m_j c_{p,j}},$$

$$(83) \qquad z = E + \hat{p} - \sum_{i=1}^{N} m_i e_{*,i},$$

$$(84) \qquad q_i = p_{\infty,i} - E + \sum_{i=1}^{N} m_i e_{*,i},$$

then g can be written in the form

$$(85) \qquad g(\hat{p}(z)) = \sum_{i=1}^{N} A_i \frac{z}{z + q_i}.$$

We consider now the function

$$(86) \qquad \varphi(z(\hat{p})) = g(\hat{p}) - 1 = \sum_{i=1}^{N} A_i \frac{z}{z + q_i} - 1,$$

subject to the constraints

$$(87) \qquad A_i \geq 0 \quad \forall i,$$

$$(88) \qquad \sum_{i=1}^{N} A_i < 1,$$

$$(89) \qquad z \in \mathcal{Z} = \left(-\min_i q_i, +\infty \right),$$

which follow from Restriction 1, Restriction 6, and Lemma 6.

Below, we will derive some results concerning solutions to (81), expressed in the form

$$(90) \qquad \varphi(z) = 0.$$

We start by making the observation that

$$(91) \qquad \frac{\mathrm{d}\varphi}{\mathrm{d}z} = \sum_{i=1}^{N} A_i \frac{q_i}{(z + q_i)^2}.$$

LEMMA 7. *If*

$$(92) \qquad \min_i q_i \geq 0,$$

the equation

$$(93) \qquad \varphi(z) = 0$$

has no solution in the interval $\mathcal{Z}$.

Proof. We first note that $\varphi(z)$ is a rational function without poles in $\mathcal{Z}$. Hence φ is C^∞-smooth in the interval $\mathcal{Z}$. We further note that from (87), (91), and (92) it follows that

$$\frac{\mathrm{d}\varphi}{\mathrm{d}z} \geq 0 \tag{94}$$

in this interval. Hence

$$\sup_{z \in \mathcal{Z}} \varphi(z) = \lim_{z \to \infty} \varphi(z) = \sum_{i=1}^{N} A_i - 1 < 0, \tag{95}$$

so no solution can exist. □

We now consider the case

$$\min_i q_i < 0. \tag{96}$$

Under this condition, $\varphi'(z)$ as given by (91) does not have a definite sign. However, a simple transformation on φ will give us a monotonic function, as stated below.

LEMMA 8. *The function $\Phi(z)$ given by*

$$\Phi : z \mapsto z\varphi(z) \tag{97}$$

is monotonicly decreasing in the interval $\mathcal{Z}$.

Proof. We first note that $\Phi(z)$, being the product of two C^∞-smooth functions, is itself C^∞-smooth in $\mathcal{Z}$. Now

$$\frac{\mathrm{d}\Phi}{\mathrm{d}z} = \varphi(z) + z\frac{\mathrm{d}\varphi}{\mathrm{d}z} = \sum_{i=1}^{N} A_i - 1 - \sum_{i=1}^{N} A_i \left(\frac{q_i}{z + q_i}\right)^2 < 0, \tag{98}$$

where we have used (87) and (88). □

PROPOSITION 3. *The equation*

$$\varphi(z) = 0 \tag{99}$$

has a solution in the interval $\mathcal{Z}$ if and only if

$$\min_i q_i < 0. \tag{100}$$

This solution is unique.

Proof. Assume first that the condition (100) is satisfied. Then all $z \in \mathcal{Z}$ satisfy $z > 0$, and $\Phi(z) = 0$ if and only if $\varphi(z) = 0$. Now

$$\lim_{z \to -\min_i q_i^+} \Phi(z) = +\infty \tag{101}$$

and

$$\lim_{z \to \infty} \Phi(z) = -\infty, \tag{102}$$

and we have already established that $\Phi(z)$ is monotonicly decreasing in $\mathcal{Z}$. Hence, by smoothness, $\Phi(z) = 0$ has precisely one solution in $\mathcal{Z}$ when (100) is satisfied. Lemma 7 completes the proof. □

We have now established sufficient results to formulate our main conclusions. First, we note that from Lemma 7 and (84) we may conclude the following.

RESTRICTION 7. *Physically valid solutions require*

$$E - \sum_{j=1}^{N} m_j e_{*,j} > \min_i p_{\infty,i}. \tag{103}$$

This leads us toward the following proposition.

PROPOSITION 4. *Problem* 2 *has a physically valid solution in the sense of Definition* 4 *if and only if E and m_i satisfy Restrictions* 6–7. *This solution is unique.*

Proof. We have shown that if a physically valid solution exists, then Restrictions 6–7 are satisfied. Assume now that Restrictions 6–7 are satisfied. Then, from (29) and (82), it follows that (87) is satisfied. Furthermore, from (29) it also follows that (88) is satisfied. Hence it follows from Proposition 3 that (90) has a unique solution in the interval $\mathcal{P}_1$.

It remains to show that this solution is physically valid, and that the full physical state is uniquely determined. Now (81) gives us directly that (63) is satisfied. Furthermore, from (29), (68), (74), (79), and (103) it follows that (62) is satisfied and that all α_i are uniquely determined. From (68), (74), (78), and (103) it follows that (65) is satisfied and that T is uniquely determined.

Finally, from (28), (29), (60), (65), and (74) it follows that (64) is satisfied and that ρ_i is uniquely determined for all i. □

4.2. Positivity of the internal energies. In this section, we wish to derive conditions under which physically valid solutions are also positive-energy solutions.

PROPOSITION 5. *A physically valid solution to Problem* 2 *is a positive-energy solution if and only if one of the following requirements is satisfied: either*

$$\min_i p_{\infty,i} \geq 0 \tag{104}$$

or
$$\left(E - \min_j (\gamma_j p_{\infty,j}) - \sum_{j=1}^{N} m_j e_{*,j} \right) \sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{p_{\infty,i} - \min_j (\gamma_j p_{\infty,j})} > \sum_{i=1}^{N} m_i c_{p,i}. \tag{105}$$

Proof. From (16), Restriction 1, and Lemma 6, it follows that a necessary and sufficient condition for a physically valid solution to be a positive-energy solution is

$$p \in \left(-\min_i (\gamma_i p_{\infty,i}), +\infty \right), \tag{106}$$

which follows directly from Lemma 6 if (104) holds.

Otherwise, write $g(\hat{p}) = 1$ as

$$\Phi(z(\hat{p})) = z \left(\sum_{i=1}^{N} A_i \frac{z}{z + q_i} - 1 \right) = 0. \tag{107}$$

Lemma 8 tells us that $\Phi(z)$ is a strictly decreasing function in the interval $\mathcal{Z}$, corresponding to

$$\hat{p} \in \left(-\min_i p_{\infty,i}, +\infty \right). \tag{108}$$

Since we now have from (83) that

$$\frac{\mathrm{d}z}{\mathrm{d}\hat{p}} \equiv 1,$$ (109)

it follows that a positive-energy solution to (107) requires

$$\Phi\left(z|\hat{p} = -\min_i\left(\gamma_i p_{\infty,i}\right)\right) = \Phi\left(E - \min_i\left(\gamma_i p_{\infty,i}\right) - \sum_{i=1}^{N} m_i e_{*,i}\right) > 0.$$ (110)

This is precisely the condition (105). Conversely, if the solution does not satisfy (106), then

$$\Phi\left(E - \min_i\left(\gamma_i p_{\infty,i}\right) - \sum_{i=1}^{N} m_i e_{*,i}\right) \leq 0. \qquad \square$$ (111)

4.3. Positivity of the pressure. Just as in section 3, our definition of physically valid solutions is sufficiently weak to allow for a negative pressure. We now consider the stronger constraint that the pressure must remain positive.

RESTRICTION 8. *A physically valid solution to Problem 2 is a strictly valid solution in the sense of Definition 4 if and only if one of the following requirements is satisfied: either*

$$\min_i p_{\infty,i} \leq 0$$ (112)

or

$$\left(E - \sum_{j=1}^{N} m_j e_{*,j}\right)\sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i}\frac{m_i c_{p,i}}{p_{\infty,i}} > \sum_{i=1}^{N} m_i c_{p,i}.$$ (113)

Proof. If (112) holds, it follows from Lemma 6 that any physically valid solution is also a strictly valid solution. Otherwise, write $g(\hat{p}) = 1$ as (107). It then follows from a line of reasoning completely similar to the proof of Proposition 5 that a positive pressure solution to (107) requires

$$\Phi(z|\hat{p} = 0) = \Phi\left(E - \sum_{i=1}^{N} m_i e_{*,i}\right) > 0.$$ (114)

This is precisely the condition (113). Conversely, if the solution satisfies $p \leq 0$, then $\Phi(E - \sum_{i=1}^{N} m_i e_{*,i}) \leq 0$. $\qquad \square$

This result may be incorporated with Proposition 4 to yield a more compact characterization of strictly valid solutions, as follows.

PROPOSITION 6. *Problem 2 has a strictly valid solution in the sense of Definition 4 if and only if E_i and m_i satisfy Restrictions 6–8. This solution is unique.*

Proof. The result follows directly from Proposition 4 and Restriction 8. $\qquad \square$

COROLLARY 1. *Problem 2 has a strictly valid, positive-energy solution in the sense of Definition 4 if and only if E_i and m_i satisfy Restrictions 6–7, and in addition one of the following is satisfied:*

   1.

$$\min_i p_{\infty,i} > 0$$ (115)

and

$$(116) \qquad \left(E - \sum_{j=1}^{N} m_j e_{*,j}\right) \sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{p_{\infty,i}} > \sum_{i=1}^{N} m_i c_{p,i},$$

2.

$$(117) \qquad \min_i p_{\infty,i} < 0$$

and

(118)
$$\left(E - \min_j (\gamma_j p_{\infty,j}) - \sum_{j=1}^{N} m_j e_{*,j}\right) \sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{p_{\infty,i} - \min_j (\gamma_j p_{\infty,j})} > \sum_{i=1}^{N} m_i c_{p,i},$$

3.

$$(119) \qquad \min_i p_{\infty,i} = 0.$$

This solution is unique.

Proof. The result follows from Proposition 4 and checking all possible signs of $\min_i p_{\infty,i}$ in Proposition 5 and Restriction 8. □

5. Numerical solution algorithms. In this section, we derive second-order solution algorithms for Problems 1 and 2. We will base our approach on the standard Newton–Raphson method. However, we want our algorithms to be unconditionally globally convergent, a property which would not be ensured if we were to use Newton's algorithm directly on the functions f and g given by (45) and (80). Instead, we will make use of the following observation.

PROPOSITION 7. *Consider the equation*

$$(120) \qquad f(x) = 0, \qquad x \in \mathcal{S} \subseteq \mathbb{R}.$$

Let $g(x)$ be some C^1-smooth function without roots in $\mathcal{S}$, and let

$$(121) \qquad f'(x) \neq 0$$

in $\mathcal{S}$. Then Newton's method applied to the function

$$(122) \qquad F(x) = f(x) \cdot g(x)$$

will yield a quadratically convergent method to a root of f, subject to the standard conditions for quadratic convergence of Newton's method applied to F. Furthermore, Newton's method applied to F will throughout $\mathcal{S}$ be a second-order accurate approximation to Newton's method applied to f.

Proof. The definition of quadratic convergence may be stated as follows:

$$(123) \qquad |x^* - x_{n+1}| \leq K|x^* - x_n|^2$$

for all x_n in some neighborhood close to x^*, where x^* is the root and K is some positive constant. Since the roots of F coincide with the roots of f, and (123) involves only the root x^*, it follows that second-order convergence for F implies second-order convergence for f.

Furthermore, Newton's method applied to f yields

(124) $$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Newton's method applied to F yields

(125)
$$\begin{aligned}
\tilde{x}_{n+1} &= x_n - \frac{f(x_n)}{f'(x_n)} \left(1 + \frac{f(x_n)g'(x_n)}{f'(x_n)g(x_n)} \right)^{-1} \\
&= x_n - \frac{f(x_n)}{f'(x_n)} \left(1 - \frac{f(x_n)g'(x_n)}{f'(x_n)g(x_n)} + \mathcal{O}(\Delta x^2) \right) \\
&= x_{n+1} + \mathcal{O}(\Delta x^2),
\end{aligned}$$

where

(126) $$\Delta x = x_{n+1} - x_n$$

and we have used that

(127) $$f(x_n) = \mathcal{O}(\Delta x). \qquad \square$$

The usefulness of this observation now lies in the possibility that a function F may be found such that the method (125) provides us with better convergence properties than the method (124). In the following, we will use this trick to obtain globally convergent methods for Problems 1 and 2.

To this end, we will use the following classic result.

PROPOSITION 8. *Consider the equation*

(128) $$F(x) = 0, \qquad x \in \mathcal{S} \subseteq \mathbb{R},$$

where $F(x)$ is at least C^2-smooth. Consider now an interval $\mathcal{T} \subseteq \mathcal{S}$, and assume that (128) has a root x^* in $\mathcal{T}$, i.e.,

(129) $$F(x^*) = 0.$$

Assume that for all $x \in \mathcal{T}$ we have

(130) $$F'(x) \neq 0,$$

(131) $$F(x) \cdot F''(x) > 0 \quad \forall x \neq x^*.$$

Then Newton's method converges monotonically and quadratically to x^* for all initial values $x_0 \in \mathcal{T}$.

The reader is referred to [18] and references therein for a review and more general convergence criteria for Newton's method. For our current purposes, Proposition 8 will be sufficient.

5.1. Problem 1. Let p^* be the pressure that solves (46), where $f(\hat{p})$ is given by (45). In the context of Proposition 8, we then have

(132) $$F_a(\hat{p}) = \sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{\hat{p} + \gamma_i p_{\infty,i}} - 1,$$

(133) $$F_a'(\hat{p}) = -\sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{(\hat{p} + \gamma_i p_{\infty,i})^2},$$

(134) $$F_a''(\hat{p}) = 2\sum_{i=1}^{N} \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{(\hat{p} + \gamma_i p_{\infty,i})^3}.$$

Newton's method gives

$$(135) \qquad \hat{p}_{n+1} = \hat{p}_n - \frac{F_a(\hat{p}_n)}{F_a'(\hat{p}_n)} = \hat{p}_n + \frac{1 - f(\hat{p}_n)}{f'(\hat{p}_n)},$$

where $f(\hat{p})$ is given by (45) and $f'(\hat{p})$ is given by (49).

LEMMA 9. *Assume that a physically valid solution p^* to Problem 1 exists. Then the method (135) converges monotonically and quadratically to p^* for all initial values satisfying*

$$(136) \qquad \hat{p}_0 \in \mathcal{P}_3, \quad where \quad \mathcal{P}_3 = \left(-\min_i (\gamma_i p_{\infty,i}), p^* \right].$$

Proof. It follows from Restriction 1, Lemma 2, and Restriction 3 that in the interval $\mathcal{P}_3$, $F_a'(\hat{p}) < 0$ and F_a is monotonically decreasing. Hence $F_a(\hat{p}) > 0$ for all $\hat{p} \neq p^*$ in this interval. Furthermore, we see from (134) that $F_a''(\hat{p}) > 0$ throughout the interval $\mathcal{P}_3$. Hence the conditions of Proposition 8 apply. □

We now turn our attention to initial values satisfying

$$(137) \qquad \hat{p}_0 \in [p^*, +\infty).$$

The method (135) then no longer satisfies the convexity requirement (131), and in general we have no guarantee that successive iterates $\hat{p}_n$ will remain in the interval $\mathcal{P}_1$ as given by (40). We will therefore make use of Proposition 7, and we consider instead the function

$$(138) \qquad F_b(\hat{p}) = \left(\hat{p} + \min_j (\gamma_j p_{\infty,j}) \right) F_a(\hat{p}).$$

We then have

$$(139) \qquad F_b'(\hat{p}) = f(\hat{p}) - 1 + \left(\hat{p} + \min_j (\gamma_j p_{\infty,j}) \right) f'(\hat{p}),$$

$$(140) \qquad \begin{aligned} F_b''(\hat{p}) &= 2f'(\hat{p}) + \left(\hat{p} + \min_j (\gamma_j p_{\infty,j}) \right) f''(\hat{p}) \\ &= 2 \sum_{i=1}^N \frac{(\gamma_i - 1)(E_i - m_i e_{*,i})}{(\hat{p} + \gamma_i p_{\infty,i})^2} \left(\frac{\hat{p} + \min_j (\gamma_j p_{\infty,j})}{\hat{p} + \gamma_i p_{\infty,i}} - 1 \right). \end{aligned}$$

Newton's method applied to F_b gives

$$(141) \quad \hat{p}_{n+1} = \hat{p}_n - \frac{F_b(\hat{p}_n)}{F_b'(\hat{p}_n)} = \hat{p}_n + \frac{1 - f(\hat{p}_n)}{f'(\hat{p}_n)} \left(1 - \frac{1 - f(\hat{p}_n)}{f'(\hat{p}_n)(\hat{p}_n + \min_j (\gamma_j p_{\infty,j}))} \right)^{-1}.$$

LEMMA 10. *Assume that a physically valid solution p^* to Problem 1 exists, and that*

$$(142) \qquad \gamma_i p_{\infty,i} = \gamma_j p_{\infty,j} = \widetilde{\gamma p_\infty} \qquad \forall i,j \in \{1, \ldots, N\}.$$

Then the method (141) converges in one step to p^* for all initial values satisfying

$$(143) \qquad \hat{p}_0 \in [p^*, +\infty).$$

Proof. When (142) holds, the method (141) reduces to

$$
(144) \qquad \hat{p}_{n+1} = \sum_{i=1}^{N} (\gamma_i - 1)(E_i - m_i e_{*,i}) - \widetilde{\gamma p_\infty} \quad \forall n.
$$

Substituting into (45) yields

$$
(145) \qquad f(\hat{p}_{n+1}) = 1. \qquad \square
$$

LEMMA 11. *Assume that a physically valid solution p^* to Problem 1 exists. Then the method* (141) *converges monotonically and at least quadratically to p^* for all initial values satisfying*

$$
(146) \qquad \hat{p}_0 \in \mathcal{P}_4, \quad where \quad \mathcal{P}_4 = [p^*, +\infty).
$$

Proof. We know from (49) that $f'(\hat{p}) < 0$ in the interval $\mathcal{P}_1$, and from this it follows that $f(\hat{p}) \leq 1$ in the interval $\mathcal{P}_4$. We then see from Restriction 1 and (138) that $F_b(\hat{p}) < 0$ for all $\hat{p} \neq p^*$ in $\mathcal{P}_4$, and from (139) that $F_b'(\hat{p}) < 0$ in this interval. Furthermore, from Restrictions 1 and 3, Lemma 1, and (140), we see that $F_b''(\hat{p}) < 0$ in $\mathcal{P}_4$, assuming that (142) does not hold. Then the conditions of Proposition 8 apply.

In the case that (142) does in fact hold, the result follows from Lemma 10. $\square$

We are now in position to formulate our globally convergent method, as follows.

PROPOSITION 9. *Assume that E_i and m_i satisfy Restrictions 2–4. Then the method*

$$
(147) \qquad \hat{p}_{n+1} = \hat{p}_n + \frac{1 - f(\hat{p}_n)}{f'(\hat{p}_n)} \left(1 - \frac{1 - f(\hat{p}_n) + |1 - f(\hat{p}_n)|}{2 f'(\hat{p}_n)(\hat{p}_n + \min_j (\gamma_j p_{\infty,j}))} \right)^{-1},
$$

where $f(\hat{p})$ is given by (45) *and $f'(\hat{p})$ is given by* (49), *converges monotonically and at least quadratically to the unique physically valid solution p^* to Problem 1 for all initial values satisfying*

$$
(148) \qquad \hat{p}_0 \in \mathcal{P}_2, \quad where \quad \mathcal{P}_2 = \left(-\min_i (\gamma_i p_{\infty,i}), +\infty \right).
$$

Proof. We know from (49) that $f(\hat{p})$ is monotonically decreasing in the interval $\mathcal{P}_2$. Hence we have $f(\hat{p}) \geq 1$ in the interval $\mathcal{P}_3$, and the method (147) reduces to (135) in this interval. Monotonicity also implies that $f(\hat{p}) \leq 1$ in the interval $\mathcal{P}_4$, and the method (147) reduces to (141) in this interval. The result now follows from Lemmas 9–11 and Proposition 1. $\square$

5.2. Problem 2. We here focus on Problem 2 as stated in section 4. Now let p^* be the pressure that solves (81), where $g(\hat{p})$ is given by (80). Consider now Newton's method applied to the function φ given by (86), where the parameters are given by (82)–(84). We obtain

$$
(149) \qquad z_{n+1} = z_n - \frac{\varphi(z_n)}{\varphi'(z_n)}.
$$

Now from (85) and (86) it follows that

$$
(150) \qquad \varphi(z) = g(\hat{p}) - 1.
$$

From (83), (109), and (150) it then follows that the method (149) can be written in the equivalent form

$$(151) \qquad \hat{p}_{n+1} = \hat{p}_n + \frac{1 - g(\hat{p}_n)}{g'(\hat{p}_n)},$$

where $g(\hat{p})$ is given by (80) and $g'(\hat{p})$ is given by

$$(152) \qquad g'(\hat{p}) = \sum_{i=1}^{N} \frac{\gamma_i - 1}{\gamma_i} \frac{m_i c_{p,i}}{\sum_{j=1}^{N} m_j c_{p,j}} \frac{p_{\infty,i} - E + \sum_{j=1}^{N} m_j e_{*,j}}{(\hat{p} + p_{\infty,i})^2}.$$

LEMMA 12. *Assume that a physically valid solution p^* to Problem 2 exists. Then the method* (151) *converges monotonically and quadratically to p^* for all initial values satisfying*

$$(153) \qquad \hat{p}_0 \in \mathcal{P}_5, \quad where \quad \mathcal{P}_5 = \left(-\min_i p_{\infty,i}, p^* \right].$$

Proof. We consider the method in the equivalent form (149), where the root z^* satisfies

$$(154) \qquad z^* = z(p^*),$$

and the condition (153) corresponds to

$$(155) \qquad z \in \left(-\min_i q_i, z^* \right].$$

Now it follows from (98) that $\varphi'(z^*) < 0$, and since z^* is the unique root that satisfies (155), it follows from continuity that

$$(156) \qquad \varphi(z) > 0 \qquad \forall z \in \left(-\min_i q_i, z^* \right).$$

Hence it follows from (98) and (100) that

$$(157) \qquad \varphi'(z) < 0 \qquad \forall z \in \left(-\min_i q_i, z^* \right].$$

Differentiating (98) yields

$$(158) \qquad \varphi''(z) = \frac{2}{z} \left(\sum_{i=1}^{N} A_i \frac{q_i^2}{(z + q_i)^3} - \varphi'(z) \right),$$

and it follows from (87), (100), and (157) that

$$(159) \qquad \varphi''(z) > 0 \qquad \forall z \in \left(-\min_i q_i, z^* \right].$$

Hence the conditions of Proposition 8 apply. □

We now focus on the interval

$$(160) \qquad \hat{p}_0 \in [p^*, +\infty).$$

As noted in section 4.1, $\varphi'(z)$ may become zero in this interval, rendering the method (151) unreliable. We therefore again make use of Proposition 7, and consider instead the function

$$(161) \qquad F_c(z) = \left(z + \min_i q_i\right) \Phi(z),$$

where Φ is given by (97). We then have

$$(162) \qquad F_c(z(\hat{p})) = \left(\hat{p} + \min_i p_{\infty,i}\right) \left(E + \hat{p} - \sum_{j=1}^{N} m_j e_{*,j}\right) (g(\hat{p}) - 1),$$

$$(163) \quad F_c'(z(\hat{p})) = \left(2\hat{p} + \min_i p_{\infty,i} + E - \sum_{j=1}^{N} m_j e_{*,j}\right) (g(\hat{p}) - 1)$$

$$+ \left(\hat{p} + \min_i p_{\infty,i}\right) \left(E + \hat{p} - \sum_{j=1}^{N} m_j e_{*,j}\right) g'(\hat{p}).$$

Newton's method applied to F_c yields

$$(164) \qquad \hat{p}_{n+1} = \hat{p}_n - \frac{F_c(z(\hat{p}_n))}{F_c'(z(\hat{p}_n))} = \hat{p}_n + \frac{1 - g(\hat{p}_n)}{g'(\hat{p}_n)} \left(1 - \frac{1 - g(\hat{p}_n)}{g'(\hat{p}_n)} h(\hat{p}_n)\right)^{-1},$$

where $h(\hat{p})$ is given by

$$(165) \qquad h(\hat{p}) = \frac{1}{E + \hat{p} - \sum_{j=1}^{N} m_j e_{*,j}} + \frac{1}{\hat{p} + \min_i p_{\infty,i}}.$$

LEMMA 13. *Assume that a physically valid solution p^* to Problem 2 exists. Then the method (164) converges monotonically and quadratically to p^* for all initial values satisfying*

$$(166) \qquad \hat{p}_0 \in \mathcal{P}_6, \quad where \quad \mathcal{P}_6 = [p^*, +\infty).$$

Proof. By Lemma 6, Lemma 8, and (83)–(84), it follows that

$$(167) \qquad F_c(z) < 0 \qquad \forall \hat{p}(z) \in (p^*, +\infty).$$

Furthermore, we have

$$(168) \qquad F_c'(z) = \left(z + \min_i q_i\right) \Phi'(z) + \Phi(z),$$

and it follows from Lemma 8 and (83)–(84) that

$$(169) \qquad F_c'(z) < 0 \qquad \forall \hat{p}(z) \in [p^*, +\infty).$$

Differentiating (168) yields

$$(170) \qquad F_c''(z) = 2\Phi'(z) + \left(z + \min_i q_i\right) \Phi''(z),$$

which by (98) can be written as

$$(171) \qquad F_c''(z) = 2 \left(\sum_{i=1}^{N} A_i - 1 + \sum_{i=1}^{N} A_i \left(\frac{q_i}{z + q_i}\right)^2 \left(\frac{z + \min_j q_j}{z + q_i} - 1\right)\right).$$

Hence

$$(172) \qquad F_c''(z) < 0 \qquad \forall \hat{p}(z) \in [p^*, +\infty) \,,$$

and the conditions of Proposition 8 apply. $\quad\square$

We may now formulate our globally convergent method, as follows.

PROPOSITION 10. *Assume that E_i and m_i satisfy Restrictions* 6–7. *Then the method*

$$(173) \qquad \hat{p}_{n+1} = \hat{p}_n + \frac{1 - g(\hat{p}_n)}{g'(\hat{p}_n)} \left(1 - \frac{1 - g(\hat{p}_n) + |1 - g(\hat{p}_n)|}{2 g'(\hat{p}_n)} h(\hat{p}_n) \right)^{-1},$$

where $g(\hat{p})$ is given by (80), *$g'(\hat{p})$ is given by* (152), *and $h(\hat{p})$ is given by* (165), *converges monotonically and quadratically to the unique physically valid solution p^* to Problem* 2, *for all initial values satisfying*

$$(174) \qquad \hat{p}_0 \in \mathcal{P}_1, \quad where \quad \mathcal{P}_1 = \left(-\min_i p_{\infty,i}, +\infty \right).$$

Proof. We know from (157) that $\varphi(z)$ is monotonically decreasing in the interval $\mathcal{P}_5$. Hence we have $g(\hat{p}) \geq 1$ in $\mathcal{P}_5$, and the method (173) reduces to (151) in this interval. In particular, we have that $\varphi'(z(p^*)) < 0$, and since p^* is the unique solution to $g(\hat{p}) = 1$ in the interval $\mathcal{P}_1$, it follows that $g(\hat{p}) \leq 1$ in the interval $\mathcal{P}_6$. Note that the method (173) reduces to (164) in this interval. The result now follows from Lemmas 12–13 and Proposition 4. $\quad\square$

6. Numerical examples. The purpose of this section is to numerically demonstrate and verify the results derived above. In particular, our examples will illustrate the quadratic and monotone convergence of our methods. We first define some useful concepts.

DEFINITION 5. *At each step of the Newton iteration, we define the* error $\mathcal{E}_n$ *as*

$$(175) \qquad \mathcal{E}_n = \hat{p}_n - p^*.$$

We also define the relative error $\mathcal{R}_n$ *as*

$$(176) \qquad \mathcal{R}_n = \left| \frac{\mathcal{E}_n}{p^*} \right|,$$

as well as the local convergence rate $\mathcal{L}_n$,

$$(177) \qquad \mathcal{L}_n = \frac{\ln |\mathcal{E}_{n+1}/\mathcal{E}_n|}{\ln |\mathcal{E}_n/\mathcal{E}_{n-1}|}.$$

The local convergence rate $\mathcal{L}$ is related to, but generally not identical to, the global convergence order. However, $\mathcal{L}_n$ will approach the global convergence order as we approach the solution.

6.1. Problem 1. We first consider Problem 1 concerning mechanical equilibria; see section 3. This corresponds to multifluid models of the kind treated, e.g., by Paillère, Corre, and García Cascales [13], and we will use their parameters corresponding to water and air as an example. Our input state and the corresponding equilibrium solution are given in Table 1, while the equation-of-state parameters can be found in Table 2. In this case, we have two fluids, $N = 2$.

TABLE 1
State variables for Problem 1.

Symbol (unit)	Value
m_1 (kg/m^3)	2.252×10^{-1}
m_2 (kg/m^3)	5.000×10^4
E_1 (J/m^3)	8.201×10^2
E_2 (J/m^3)	1.058×10^9
α_1 (−)	0.200
α_2 (−)	0.800
p (MPa)	0.100
T_1 (K)	308.15
T_2 (K)	308.15

TABLE 2
EOS parameters for Problem 1.

	γ_j (−)	$p_{\infty,j}$ (Pa)	$c_{p,j}$ (J/(kg K))	$e_{*,j}$ (J/(kg))
gas (1)	1.4	0	1008.7	0
liquid (2)	2.8	8.5×10^8	4186.0	0

TABLE 3
Convergence for Problem 1 *with* $\hat{p}_0 = 1 \times 10^4$ Pa.

n	$\hat{p}_n$ (Pa)	$\mathcal{E}_n$ (Pa)	$\mathcal{R}_n$ (−)	$\mathcal{L}_n$
0	1.000×10^4	-9.00×10^4	9.00×10^{-1}	−
1	1.900×10^4	-8.10×10^4	8.10×10^{-1}	2.00
2	3.439×10^4	-6.56×10^4	6.56×10^{-1}	2.00
3	5.695×10^4	-4.30×10^4	4.30×10^{-1}	2.00
4	8.147×10^4	-1.85×10^4	1.85×10^{-1}	2.00
5	9.656×10^4	-3.43×10^3	3.43×10^{-2}	2.00
6	9.988×10^4	-1.17×10^2	1.17×10^{-3}	2.00
7	1.000×10^5	-1.38×10^{-1}	1.38×10^{-6}	2.00
8	1.000×10^5	-1.92×10^{-7}	1.92×10^{-12}	2.00
9	1.000×10^5	-3.70×10^{-19}	3.70×10^{-24}	−

We employ the method (147) of Proposition 9. The results are shown in Table 3 for

$$\hat{p}_0 = 1 \times 10^4 \, \text{Pa} < p^*, \tag{178}$$

and in Table 4 for

$$\hat{p}_0 = 1 \times 10^{12} \, \text{Pa} > p^*. \tag{179}$$

We observe the expected quadratic convergence, and the monotonicity is verified by $\mathcal{E}_n$ having a constant sign.

The results from Tables 3–4 are graphically illustrated in Figure 1. Figure 1(a) contains the function F_a given by (132), and Figure 1(b) contains the function F_b given by (138). As described in section 5.1, the method (147) is equivalent to the standard Newton–Raphson algorithm applied to these functions. The figure indicates how the established convexity properties ensure the monotone convergence.

Note that for the initial value (178), the unmodified Newton–Raphson method (135) would fail. In particular, the method gives $\hat{p}_1 = -5.2 \times 10^{14}$ Pa and rapidly

TABLE 4
Convergence for Problem 1 *with* $\hat{p}_0 = 1 \times 10^{12}$ Pa.

n	$\hat{p}_n$ (Pa)	$\mathcal{E}_n$ (Pa)	$\mathcal{R}_n$ (−)	$\mathcal{L}_n$
0	1.000×10^{12}	1.00×10^{12}	1.00×10^{7}	–
1	1.895×10^{9}	1.89×10^{9}	1.89×10^{4}	0.21
2	4.975×10^{8}	4.97×10^{8}	4.97×10^{3}	1.03
3	1.257×10^{8}	1.25×10^{8}	1.25×10^{3}	1.45
4	1.731×10^{7}	1.72×10^{7}	1.72×10^{2}	1.82
5	5.642×10^{5}	4.64×10^{5}	4.64×10^{0}	1.98
6	1.003×10^{5}	3.61×10^{2}	3.61×10^{-3}	2.00
7	1.000×10^{5}	2.19×10^{-4}	2.19×10^{-9}	2.00
8	1.000×10^{5}	8.09×10^{-17}	8.09×10^{-22}	–

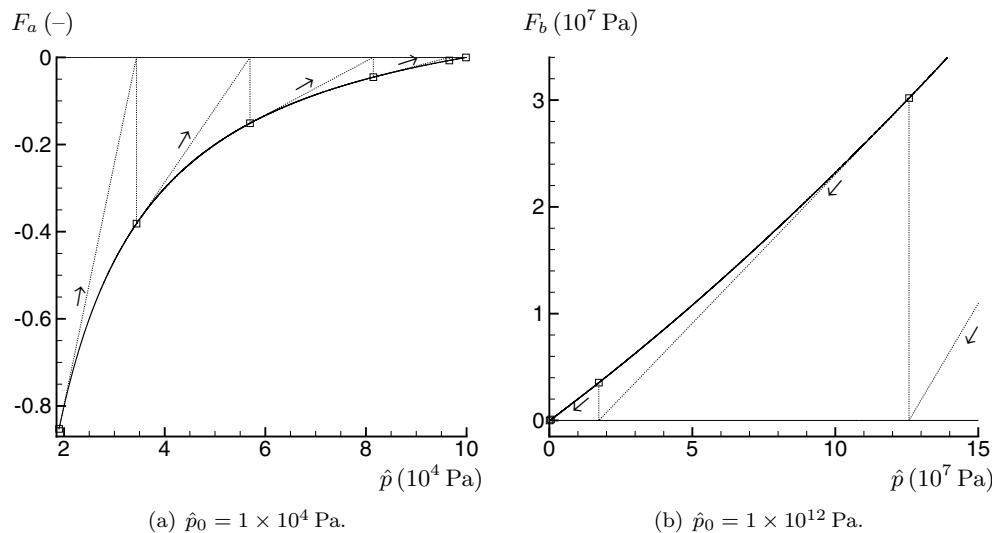(a) $\hat{p}_0 = 1 \times 10^4$ Pa.   (b) $\hat{p}_0 = 1 \times 10^{12}$ Pa.

FIG. 1. *Convergence for Problem* 1 *with the initial value lower (left) and higher (right) than the solution. The arrows indicate the direction of successive iterates.*

diverges. This shows that our modification (147) is in fact *necessary* to obtain global convergence.

6.2. Problem 2. We now consider Problem 2 with mechanical and thermal equilibria; see section 4. As an example we will take the three-component ($N = 3$) mixture whose decompression was studied by Morin et al. [9]. The input state and the corresponding equilibrium solution are shown in Table 5, while the equation-of-state parameters are given in Table 6.

The numerical algorithm (173) of Proposition 10 has been applied. Table 7 shows the result for an initial pressure of

$$\text{(180)} \qquad \hat{p}_0 = - \min_j p_{\infty,j} = -1.094 \times 10^7 \,\text{Pa} < p^*,$$

while Table 8 presents results for an initial pressure of

$$\text{(181)} \qquad \hat{p}_0 = 1 \times 10^{10} \,\text{Pa} > p^*.$$

Again the expected convergence order and monotonicity are verified.

TABLE 5
State variables for Problem 2.

Symbol (unit)	Value
m_1 (kg/m^3)	6.235×10^2
m_2 (kg/m^3)	9.378×10^1
m_3 (kg/m^3)	1.274×10^0
E (J/m^3)	8.332×10^8
α_1 (−)	0.9
α_2 (−)	0.09
α_3 (−)	0.01
p (MPa)	10
T (K)	300

TABLE 6
EOS parameters for Problem 2.

	γ_j (−)	$p_{\infty,j}$ (MPa)	$c_{p,j}$ (J/(kg K))	$e_{*,j}$ (J/(kg))
CO$_2$ (1)	1.03	13.47	3877	0
Water (2)	2.85	833.02	4155	0
Methane (3)	1.23	10.94	2930	0

TABLE 7
Convergence for Problem 2 *with* $\hat{p}_0 = -1.094 \times 10^7$ Pa.

n	$\hat{p}_n$ (Pa)	$\mathcal{E}_n$ (Pa)	$\mathcal{R}_n$ (−)	$\mathcal{L}_n$
0	-1.094×10^7	-2.09×10^7	2.09×10^0	−
1	-1.093×10^7	-2.09×10^7	2.09×10^0	2.44
2	-1.092×10^7	-2.09×10^7	2.09×10^0	2.98
3	-1.089×10^7	-2.08×10^7	2.08×10^0	4.35
4	-1.074×10^7	-2.07×10^7	2.07×10^0	6.83
5	-9.791×10^6	-1.97×10^7	1.97×10^0	3.38
6	-6.875×10^6	-1.68×10^7	1.68×10^0	2.05
7	-2.170×10^6	-1.21×10^7	1.21×10^0	2.00
8	3.676×10^6	-6.32×10^6	6.32×10^{-1}	2.00
9	8.293×10^6	-1.70×10^6	1.70×10^{-1}	2.00
10	9.875×10^6	-1.24×10^5	1.24×10^{-2}	2.00
11	9.999×10^6	-6.59×10^2	6.59×10^{-5}	2.00
12	1.000×10^7	-1.85×10^{-2}	1.85×10^{-9}	2.00
13	1.000×10^7	-1.46×10^{-11}	1.46×10^{-18}	−

In Figure 2, the results of Tables 7–8 are represented graphically. The function φ, as given by (150), is presented in Figure 2(a) for the initial value (180). For the initial value (181), Figure 2(b) contains the function F_c as given by (162). As described in section 5.2, the method (173) reduces to the standard Newton–Raphson algorithm applied to these functions. The graphs demonstrate behavior similar to that observed for Problem 1.

As for Problem 1, we observe that the unmodified Newton–Raphson method (151) fails for the initial value (181). It gives $\hat{p}_1 = -4.2 \times 10^{12}$ Pa, and then rapidly diverges toward negative infinity. This is due to the unfavorable curvature of φ for $\hat{p} > p^*$, causing the naïve method (151) to cut through the physically relevant part of φ and give a very large negative $\hat{p}_1$. From this there is no recovery.

This underscores the necessity of our modification (173).

TABLE 8
Convergence for Problem 2 *with* $\hat{p}_0 = 1 \times 10^{10}$ Pa.

n	$\hat{p}_n$ (Pa)	$\mathcal{E}_n$ (Pa)	$\mathcal{R}_n$ (−)	$\mathcal{L}_n$
0	1.000×10^{10}	9.99×10^9	9.99×10^2	−
1	4.803×10^9	4.79×10^9	4.79×10^2	1.06
2	2.213×10^9	2.20×10^9	2.20×10^2	1.12
3	9.357×10^8	9.25×10^8	9.25×10^1	1.23
4	3.290×10^8	3.19×10^8	3.19×10^1	1.42
5	8.005×10^7	7.00×10^7	7.00×10^0	1.60
6	1.621×10^7	6.20×10^6	6.20×10^{-1}	1.51
7	1.016×10^7	1.60×10^5	1.60×10^{-2}	1.90
8	1.000×10^7	1.59×10^2	1.59×10^{-5}	2.00
9	1.000×10^7	1.58×10^4	1.58×10^{-11}	2.00
10	1.000×10^7	1.58×10^{16}	1.58×10^{-23}	−

(a) $\hat{p}_0 = -1.094 \times 10^7$ Pa.

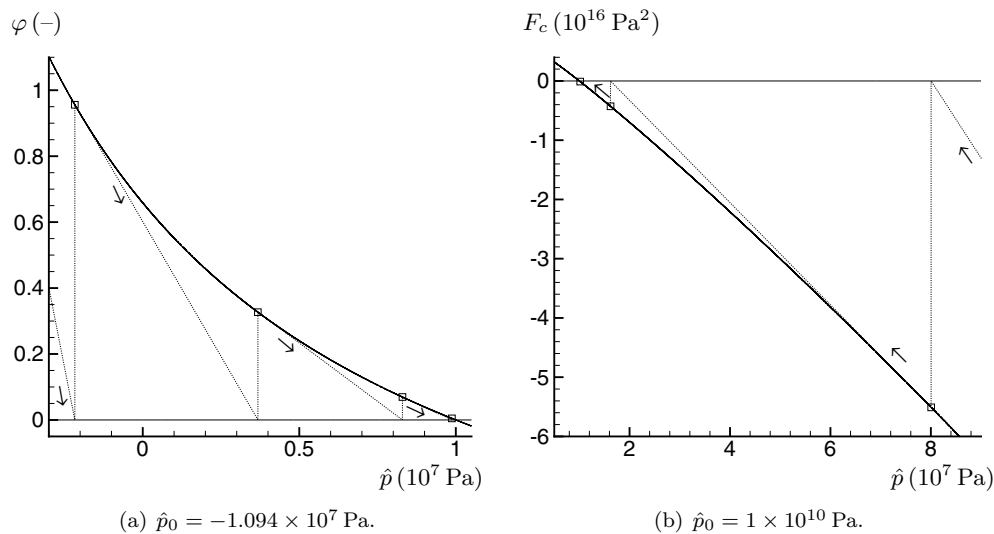(b) $\hat{p}_0 = 1 \times 10^{10}$ Pa.

FIG. 2. *Convergence for Problem* 2 *with the initial value lower (left) and higher (right) than the solution. The arrows indicate the direction of successive iterates.*

7. Summary. We have investigated a general system of N immiscible stiffened gases assumed to be in mechanical equilibrium, meaning that the pressure is identical for all the components. We have considered two cases, one in which the fluids are assumed to have individual temperatures and one in which thermal equilibrium has been assumed.

Under these assumptions, we have considered the problem of calculating the full physical state from knowledge of only the conserved fluid-mechanical parameters. To as large an extent as possible, we have attempted to give a complete exposition of this problem. We have provided some natural definitions of what *physical validity* means for such equilibrium solutions. We have then given the necessary and sufficient conditions for such valid solutions to exist, and we have proved that these solutions are unique.

Finally, we have demonstrated that the problems may be reduced to solving an equation in one unknown. This allows for the construction of robust and efficient

numerical solvers. In particular, we have formulated explicit Newton–Raphson-type methods which guarantee unconditional quadratic convergence.

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