A REGULARIZED STIFFENED-GAS EQUATION OF STATE

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Dedicated to Claude-Michel Brauner on the occasion of his 70th birthday.

Abstract An alternative to the stiffened-gas equation of state is proposed that corrects for unphysical behavior, namely the returning of negative pressure values for densities lower than the reference density. The question of generalizing a given isentropic equation of state is first addressed. Then, a regularized stiffened-gas equation of state is derived, which is the main goal of this work. Finally, the use of the new equation of state is briefly illustrated for a classical computational fluid dynamics benchmark concerning the evaluation of liquid impact on a wall.

Keywords Stiffened-gas, equation of state, computational fluid dynamics, slightly compressible fluid.

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1. Introduction

In numerous CFD^* applications it is necessary to handle slightly compressible fluids like liquids. Furthermore, some liquid flows with very high pressures (from tens to thousands of bars) are sometimes of interest. *E.g.* propagation of shock waves generated by underwater explosions, where liquids become fully compressible.

For divariant fluids (a substance is divariant when all its thermodynamic properties can be expressed by two independent parameters e.g. pressure and temperature), compressible solvers need Equations of State (EoS) that are generally physical laws of the form (p denotes the pressure and T the temperature):

thermodynamic function = function of
$$(p, T)$$
, (1.1)

which are either given by analytical expressions or numerical tables, for which the reader is referred to Labourdette et al. [10] and references therein.

This paper focuses on CFD solvers that use the following thermodynamic variables: ρ , e and s (respectively density, specific internal energy and specific entropy). Hence, the following functions are needed:

$$\rho = \mathcal{R}(p,T), e = \mathcal{E}(p,T), s = \mathcal{S}(p,T).$$
(1.2)

In CFD, the classical EoS is:

$$p = (\gamma - 1) \rho e, \qquad (1.3)$$

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^{*}A glossary of abbreviations used is provided for the reader before the References.

where $\gamma > 1$ is a constant. This law, known as the polytropic gas EoS, is used to close the usual conservative compressible Euler Equations, for example. In the CFD literature (1.3) was extended in the early seventies (Harlow and A. Amsden [9]) in order to represent the behavior of liquids (Water, liquefied Methane, ...) at pressure values near to 1 Bar, as follows:

$$p = (\gamma - 1) \rho e - \pi_0, \qquad (1.4)$$

where π_0 is a **constant** that depends on the liquid. Since, it has been used by many authors, see *e.g.* Saurel and Abgrall [14] and Bernard *et al.* [2], in CFD solvers.

In this paper an alternative to the SG EoS (1.4) is proposed that revises its unphysical behavior (see the numerical example at the beginning of Section 2.2). In the next Section we focus on the isentropic version of (1.4), the ISG EoS, and we first correct its unphysical behavior: production of negative pressures for densities lower than the reference density. This modification of the ISG EoS does not affect its values for densities greater than the reference density. Then, in the next Section, the general question of extending a given isentropic EoS to a general one (Theorem 3.1) is addressed. Section 4 applies this result to the IRSG EoS in order to produce the RSG EoS, which is the main goal of this work. Finally, the use of this new EoS is briefly illustrated for a classical benchmark in CFD that concerns the evaluation of liquid impacts against a wall.

2. On the classical Stiffened-Gas EoS

The usual method used to determine π_0 in (1.4) is based on the following result:

Lemma 2.1. For an EoS of the form $p = \mathcal{P}(\rho, e)$, the speed of sound (SoS) is given by:

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2} \left(\frac{\partial p}{\partial e}\right)_\rho}.$$
(2.1)

Proof. The SoS is given by:

$$c = \sqrt{\left(\frac{\partial p}{\partial \rho}\right)_s}.$$
(2.2)

Hence, we can write:

$$dp = c^2 d\rho + \left(\frac{\partial p}{\partial s}\right)_{\rho} ds. \qquad (2.3)$$

Now according to Gibbs relation:

$$Tds = de - \frac{p}{\rho^2} d\rho , \qquad (2.4)$$

so that we have:

$$dp = c^2 d\rho + \frac{de - \frac{p}{\rho^2} d\rho}{T} \left(\frac{\partial p}{\partial s}\right)_{\rho}.$$
 (2.5)

It is deduced that $\frac{1}{T} \left(\frac{\partial p}{\partial s} \right)_{\rho} = \left(\frac{\partial p}{\partial e} \right)_{\rho}, c^2 = \left(\frac{\partial p}{\partial \rho} \right)_e + \frac{p}{T \rho^2} \left(\frac{\partial p}{\partial s} \right)_{\rho}$ and (2.1) follows.

For the EoS (1.4), formula (2.1) leads to:

$$c^2 = \frac{\gamma \, p + \pi_0}{\rho} \,, \tag{2.6}$$

so that knowing, given a pressure p_0 and temperature T_0 , the values of density ρ_0 and SoS c_0 , we can find:

$$\pi_0 = \rho_0 \, c_0^2 - \gamma \, p_0 \,. \tag{2.7}$$

In this formula γ (the analogue of the adiabatic index in (1.3)) has still to be determined. As we shall see, the value of γ does not play a role. Let us consider water in normal ambient conditions, where $\rho_0 \approx 1\,000\,kg\,m^{-3}$, $c_0 \approx 1\,500\,m\,s^{-1}$ at $p_0 = 10^5 \,Pa$ and $T_0 = 300\,K$. We have $\rho_0 c_0^2 \approx 2.25\,10^9 \,Pa$, hence $\rho_0 c_0^2 \gg p_0$ and since $\gamma = \mathcal{O}(1)$, $\rho_0 c_0^2 \gg \gamma p_0$. Therefore, it can be concluded that $\pi_0 \approx \rho_0 c_0^2$ and that the numerical value of γ should not play an important role. Later, we will return to this point with a more rigorous proof, see Proposition 2.1.

2.1. The isentropic case

By assuming that the heat capacity at constant volume C_V is constant, that is:

$$C_V \equiv \left(\frac{\partial e}{\partial T}\right)_{\rho} > 0 \text{ is constant}, \qquad (2.8)$$

it is shown in the Appendix (Section 6) that combining (1.4) and (2.4) with (2.8) leads to the following expression for the specific entropy function s, as a function of p and ρ :

$$(\gamma - 1) T_0 \rho_0 C_V \left(\exp\left(\frac{s - s_0}{C_V}\right) - 1 \right) = \left(\frac{\rho}{\rho_0}\right)^{-\gamma} \left[p + \frac{\pi_0}{\gamma} \right] - \left[p_0 + \frac{\pi_0}{\gamma} \right], \quad (2.9)$$

so that the isentropic version of (1.4) is:

$$p = \left(p_0 + \frac{\pi_0}{\gamma}\right) \left(\frac{\rho}{\rho_0}\right)^{\gamma} - \frac{\pi_0}{\gamma}.$$
 (2.10)

This law is mostly known as the Isentropic Stiffened-Gas Equation (ISG), but sometimes in the literature it is referred to as Tait's law (see *e.g.* Oger *et al.* [12]).

Introducing the following non-dimensional number that quantifies the compressibility of the fluid:

$$\chi_0 \equiv \frac{p_0}{\rho_0 c_0^2} \,, \tag{2.11}$$

it is observed that (2.10) can also be written as:

$$\rho = \rho_0 \left(1 + \gamma \,\chi_0 \, \frac{p - p_0}{p_0} \right)^{1/\gamma} \,. \tag{2.12}$$

 χ_0 is very small for liquids, *e.g.* for water in ambient conditions $\chi_0 \sim 1/22500 \sim 4.44 \times 10^{-5}$, so that (2.12) can be expanded as:

$$\rho = \rho_0 \left(1 + \chi_0 \frac{p - p_0}{p_0} - \frac{\gamma - 1}{2} \left(\chi_0 \frac{p - p_0}{p_0} \right)^2 + \mathcal{O}\left(\left(\chi_0 \frac{p - p_0}{p_0} \right)^3 \right) \right). \quad (2.13)$$

Hence, over a wide range of pressure (2.10) is well approximated by the linear law:

$$\rho = \rho_0 \left(1 + \chi_0 \, \frac{p - p_0}{p_0} \right) \,, \qquad \chi_0 \equiv \frac{p_0}{\rho_0 c_0^2} \,, \tag{2.14}$$

which is independent of γ and is in fact equivalent to (2.10) for $\gamma = 1$. So it has been shown:

Proposition 2.1. For $\chi_0 \ll 1$ the ISG (2.10) is negligibly dependent on γ and is well approximated by (2.14).

2.2. Study of the ISG EoS (2.10)

However, although the ISG is used extensively in the CFD literature, it has a major drawback: it produces (non-physical) negative pressures, as is now shown in the most used case, namely water in ambient conditions.

Numerical example As already discussed, for liquids with $\gamma > 1$ the value of γ does not play a role as long as it is of order 1. Hence, $\gamma = 2$ is taken to fit (2.10) for water in conditions close to ambient. Taking $\rho_0 = 1000 \, kg \, m^{-3}$, $c_0 = 1500 \, m \, s^{-1}$ at $p_0 = 10^5 \, Pa$ we find $\pi_0 = 2.2498 \, 10^9 \, Pa$.

Now, if this numerical value is used to compute the pressure corresponding to the density $999.9 kg m^{-3}$, a negative value is found: -349958 Pa!

Discussion One might reply that, in the case of a compression, which is important when dealing with underwater explosions, the density will increase and the law (2.10) will not return negative pressures. In fact the situation is more subtle, especially in the case of compressions found when using CFD. Indeed, behind a shock wave compression there is always a depression (this is the classical solution to Riemann's Problem, Courant and Friedrichs [7]), and negative pressures are therefore produced by the law (2.10). In such a situation some code developers use so-called clipping techniques which consists of fixing a minimal value to the density, ρ_{min} for which the pressure given by the law (2.10) is positive. This technique is not acceptable in the context of *Finite Volume* CFD Codes (which are now the Sate of the Art techniques in CFD see *e.g.* the ANSYS Fluent User Guide [1] and the OpenFOAM User Guide [13]) because mass conservation is violated when clipping techniques are used.

Conclusion Law (2.10) must be modified for densities smaller than ρ_0 , *e.g.* for $\rho \leq \rho_0/2$, so that the pressure remains positive for all density values.

2.3. Regularizing the isentropic Stiffened-Gas EoS

Two simple principles are relied upon in order to build the IRSG (Isentropic Regularized Stiffened-Gas) EoS and use it for CFD simulations (see Section 5). Firstly, for vanishing pressure, according to physical considerations, all fluids behave like a perfect gas, hence we shall take:

$$p \text{ proportional to } \rho^{\gamma}, \text{ as } \rho \to 0,$$
 (2.15)

with $\gamma = 2$, (again the value of $\gamma > 1$ has very little effect).

Secondly, it is undesirable to introduce artificial discontinuities in the SoS (as these induce numerical artifacts, such as reflexions of waves, etc.), so it is imposed that the IRSG, written as:

$$p = P_{IRSG}(\rho) \equiv p_0 \varphi\left(\frac{\rho}{\rho_0}\right),$$
 (2.16)

is a smooth function (at least C^1) of ρ .

As already seen, it is only necessary to modify the original ISG EoS (2.10) for densities lower than ρ_0 , which leads us to propose the following expression for φ in (2.16) ($r_0 = 1/2$ in what follows):

$$\varphi: r \mapsto \begin{vmatrix} \varphi_0(r) = 1 + \frac{r^{\gamma} - 1}{\gamma \chi_0}, & \text{for } r \ge r_0, \\ \varphi_1(r) = \frac{\chi_0}{2r_0} \frac{r^2}{(\alpha_0 + \chi_0) r_0 - \alpha_0 r}, & \text{for } r \le r_0, \end{vmatrix}$$
(2.17)

where:

$$\chi_0 = \frac{p_0}{\rho_0 c_0^2}, \quad \text{and} \quad \alpha_0 \equiv 2 - (\gamma + 2) \,\chi_0.$$
(2.18)

Figures 1 and 2 compare both ISG and IRSG with data for liquid methane at 1 bar and with a saturation temperature $\approx 111 K$.



Figure 1. Isentropic Stiffened-Gas EoS compared with Isentropic Regularized Stiffened-Gas EoS.

3. The lift problem for a general EoS

3.1. Problem specification

Starting with an arbitrary isentropic EoS

$$p = Q(\rho), \quad \rho \ge 0, \tag{3.1}$$

with the goal to find a lift $P(\rho, s) > 0$ that is a law, such that:

$$P(\rho, s_0) = Q(\rho), \quad \forall \rho > 0, \qquad (3.2)$$



Figure 2. Isentropic Stiffened-Gas EoS compared with Isentropic Regularized Stiffened-Gas EoS (Zoom).

where s_0 denotes the reference value of the specific entropy corresponding to (3.1).

This problem has an infinite number of solutions, but some constraints apply because $P(\rho, s)$ must be a physical law, as will now discussed. Since (3.1) is a physical law, we have:

$$Q'(\rho) > 0, \quad \rho > 0,$$
 (3.3)

and for the same reason (existence of the SoS given by (2.2)) it must be the case that:

$$\left(\frac{\partial P}{\partial \rho}\right)_{s}(\rho,s) > 0, \quad \forall \rho > 0, \quad \forall s > 0.$$
(3.4)

We also have (recall that e denotes the specific internal energy):

$$P(\rho, e) > 0, \quad \forall e > 0, \quad \forall \rho > 0.$$

$$(3.5)$$

3.2. A general result

The goal of this Section is to prove the following result.

Theorem 3.1. Let Q be a given isentropic EoS (Q is a C^1 positive and strictly increasing function) that corresponds to the reference state $s = s_0$, $e = e_0 > 0$, $T = T_0 > 0$. For the two hypotheses:

$$\left(\frac{\partial e}{\partial T}\right)_{\rho}(\rho,T) \text{ is constant, } P(\rho,e=0) = 0, \quad \forall \rho > 0, \qquad (3.6)$$

one and only one law $P(\rho, s)$ exists that is a lift of (3.1), such that:

$$P(\rho, s_0) = Q(\rho), \quad \forall \rho > 0.$$
(3.7)

This is given by:

$$P(\rho, s) = Q(\rho) \exp\left(\frac{s - s_0}{C_V}\right), \qquad (3.8)$$

$$P(\rho, e) = \frac{Q(\rho)e}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr},$$
(3.9)

$$\exp\left(\frac{s(\rho, e) - s_0}{C_V}\right) = \frac{e}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr},$$
(3.10)

$$T(\rho, e) = \frac{e}{C_V}, \text{ where } C_V = \frac{e_0}{T_0}.$$
 (3.11)

The proof of this result arises from the following two propositions whose proofs are postponed until later.

Proposition 3.1. Condition (2.8) is equivalent to: a function $\theta : \mathbb{R}_+ \to \mathbb{R}_+$ exists such that:

$$T(\rho, s) = \theta(\rho) \exp\left(\frac{s - s_0}{C_V}\right).$$
(3.12)

Proposition 3.2. For condition (2.8) and having (3.7), then:

$$e(\rho, s) = C_V \,\theta(\rho) \left[\exp\left(\frac{s - s_0}{C_V}\right) - 1 \right] + e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} \, dr \,, \tag{3.13}$$

$$P(\rho, s) = C_V \rho^2 \theta'(\rho) \left[\exp\left(\frac{s - s_0}{C_V}\right) - 1 \right] + Q(\rho).$$
(3.14)

Proof of Theorem 3.1. According to (3.6) we have (3.12), (3.13) and (3.14). Denoting $s^*(\rho) := s(\rho, e = 0)$ in view of (3.13), we can write:

$$1 - \exp\left(\frac{s^*(\rho) - s_0}{C_V}\right) = \frac{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr}{C_V \,\theta(\rho)}, \qquad (3.15)$$

so that according to (3.14):

$$P(\rho, e = 0) = Q(\rho) - \frac{\rho^2 \theta'(\rho)}{\theta(\rho)} \left(e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr \right), \qquad (3.16)$$

and now $P(\rho, e = 0) = 0$ becomes:

$$\frac{\theta'(\rho)}{\theta(\rho)} = \frac{\frac{Q(\rho)}{\rho^2}}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr} \,.$$
(3.17)

This differential equation has a unique solution $(\theta(\rho_0) = T_0)$:

$$\theta(\rho) = T_0 \left(1 + \frac{1}{e_0} \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} \, dr \right). \tag{3.18}$$

It is deduced from (3.13) that

$$\exp\left(\frac{s(\rho, e) - s_0}{C_V}\right) = 1 + \frac{e_0}{C_V T_0} \frac{e - e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr},$$
(3.19)

so, returning to (3.13) and (3.14), it is found that:

$$P(\rho, e) = \frac{Q(\rho)e}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr},$$
(3.20)

and

$$T(\rho, e) = T(e) = \frac{e}{C_V}.$$
 (3.21)

Hence:

$$e_0 = C_V T_0,$$
 (3.22)

so that (3.19) yields:

$$\exp\left(\frac{s(\rho, e) - s_0}{C_V}\right) = \frac{e}{e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} dr},$$
(3.23)

and Theorem 3.1 is proved.

Proof of Proposition 3.1. By observing that according to Gibbs relation (2.4), we have:

$$\left(\frac{\partial e}{\partial s}\right)_{\rho} = T, \quad \left(\frac{\partial e}{\partial \rho}\right)_{s} = \frac{P(\rho, s)}{\rho^{2}},$$
(3.24)

(i) Assuming that (2.8) is true, according to (2.4):

$$\left(\frac{\partial T}{\partial s}\right)_{\rho} = \left(\frac{\partial T}{\partial e}\right)_{\rho} \left(\frac{\partial e}{\partial s}\right)_{\rho} = T\left(\frac{\partial T}{\partial e}\right)_{\rho} = \frac{T}{C_{v}},$$

hence (3.12) follows.

(ii) Conversely, if (3.12) is true, then

$$\left(\frac{\partial e}{\partial T}\right)_{\rho} = \frac{\left(\frac{\partial e}{\partial s}\right)_{\rho}}{\left(\frac{\partial T}{\partial s}\right)_{\rho}} = \frac{T}{\left(\frac{\partial T}{\partial s}\right)_{\rho}} = C_v \,.$$

Proof of Proposition 3.2. Taking ρ_0 as an arbitrary reference value and denoting the values of $e(\rho_0, s_0)$ and $T(\rho_0, s_0)$ by:

$$e_0 = e(\rho_0, s_0), \quad T_0 = T(\rho_0, s_0).$$
 (3.25)

According to (3.12) and (3.24) we have:

$$\left(\frac{\partial e}{\partial s}\right)_{\rho} = T = \theta(\rho) \, \exp\left(\frac{s - s_0}{C_v}\right) \,. \tag{3.26}$$

It follows that:

$$e(\rho, s) = C_v \,\theta(\rho) \,\exp\left(\frac{s - s_0}{C_v}\right) + E(\rho)\,,\tag{3.27}$$

where E is an arbitrary function which, according to (3.25), satisfies:

$$E(\rho_0) = -C_v T_0 + e_0 \,. \tag{3.28}$$

It is deduced from (3.24) that,

$$P(\rho, s) = \rho^2 \left(\frac{\partial e}{\partial \rho}\right)_s = C_v \,\rho^2 \,\theta'(\rho) \,\exp\left(\frac{s - s_0}{C_v}\right) + \rho^2 \,E'(\rho)\,,\tag{3.29}$$

so that with (3.7):

$$C_v \rho^2 \theta'(\rho) + \rho^2 E'(\rho) = Q(\rho).$$
 (3.30)

It then follows from (3.28) that

$$E(\rho) = e_0 - C_v \,\theta(\rho) + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} \,dr \,.$$
(3.31)

Hence, returning to (3.27):

$$e(\rho, s) = C_v \,\theta(\rho) \left[\exp\left(\frac{s - s_0}{C_v}\right) - 1 \right] + e_0 + \int_{\rho_0}^{\rho} \frac{Q(r)}{r^2} \, dr \,. \tag{3.32}$$

Then according to (3.29), it is found that:

$$P(\rho,s) = C_v \rho^2 \theta'(\rho) \left[\exp\left(\frac{s-s_0}{C_v}\right) - 1 \right] + Q(\rho).$$
(3.33)

3.3. On the key functions appearing in Finite Volumes Codes

In Finite Volumes Codes, that include the total energy conservation equation, the thermodynamic relation $p = P(\rho, e)$ is commonly used. Then, the two thermodynamic functions:

$$\left(\frac{\partial p}{\partial \rho}\right)_{s}(\rho, e) \quad \text{and} \quad \frac{1}{\rho T(\rho, e)} \left(\frac{\partial p}{\partial s}\right)_{\rho},$$
(3.34)

appear to be useful. The first of these is the SoS squared:

$$c^{2} = \left(\frac{\partial p}{\partial \rho}\right)_{s}(\rho, e), \qquad (3.35)$$

while the second is Grüneisen's coefficient:

$$k = \frac{1}{\rho T(\rho, e)} \left(\frac{\partial p}{\partial s}\right)_{\rho}.$$
(3.36)

For the hypotheses given in Theorem 3.1, we then have:

$$c^{2}(\rho, e) = Q'(\rho) \frac{e}{e_{0} + \int_{\rho_{0}}^{\rho} \frac{Q(r)}{r^{2}} dr}, \quad k(\rho, e) = k(\rho) = \frac{Q(\rho)}{\rho \left(e_{0} + \int_{\rho_{0}}^{\rho} \frac{Q(r)}{r^{2}} dr\right)}.$$
 (3.37)

4. Application to the Stiffened-Gas EoS

In this Section the objective is to build a generalization of the SG EoS (1.4) that ensures a positive pressure. In Section 2.3 a regularized version of the ISG EoS was constructed, as given by (2.16)-(2.17), which is the IRSG. Now we are going to use Theorem 3.1 to find a lift of the IRSG.

Let then Q be given by (2.16)-(2.17). In view of (3.9)-(3.10), we need to compute the integral:

$$I(\rho) = \int_{\rho_0}^{\rho} \frac{Q(s)}{s^2} ds = \frac{p_0}{\rho_0} \underbrace{\int_1^r \frac{\varphi(s)}{s^2} ds}_{\equiv J(r)}, \quad r = \frac{\rho}{\rho_0}.$$
 (4.1)

It can be seen that the computations need to be done in two steps by observing that $r_0 < 1$ and that φ has two different expressions according to the position of r with respect to r_0 .

For $r \ge r_0$. An easy computation shows that (for $\gamma > 1$):

$$J(r) = \left(1 - \frac{1}{\chi_0 \gamma}\right) \left(1 - \frac{1}{r}\right) + \frac{r^{\gamma - 1} - 1}{\chi_0 \gamma(\gamma - 1)}, \quad \forall r \ge r_0.$$

$$(4.2)$$

For $r \leq r_0$. In this case we write:

$$J(r) = \int_{1}^{r_0} \frac{\varphi_0(s)}{s^2} \, ds + \int_{r_0}^{r} \frac{\varphi_1(s)}{s^2} \, ds \,. \tag{4.3}$$

The first integral has already been computed, while for the second:

$$\int_{r_0}^r \frac{\varphi_1(s)}{s^2} ds = \frac{\chi_0}{2r_0} \ln\left(\frac{\chi_0 r_0}{(\alpha_0 + \chi_0)r_0 - \alpha_0 r}\right).$$
(4.4)

Finally the function $I(\rho)$, (4.1), appearing in (3.9)-(3.10) is:

$$I(\rho) = \begin{cases} \frac{p_0}{\rho_0} \left[\left(1 - \frac{1}{\chi_0 \gamma}\right) \left(1 - \frac{1}{r}\right) + \frac{r^{\gamma - 1} - 1}{\chi_0 \gamma(\gamma - 1)} \right], \text{ for } r \leq r_0, \\ \frac{p_0}{\rho_0} \left[\left(1 - \frac{1}{\chi_0 \gamma}\right) \left(1 - \frac{1}{r_0}\right) + \frac{r_0^{\gamma - 1} - 1}{\chi_0 \gamma(\gamma - 1)} + \frac{\chi_0}{2r_0} \ln\left(\frac{\chi_0 r_0}{(\alpha_0 + \chi_0)r_0 - \alpha_0 r}\right) \right], \text{ for } r \geq r_0. \end{cases}$$

Figures 3 and 4 show the SG and RSG laws.



Figure 3. Comparison of SG and RSG laws.

In Figure 4 it is observed that the regularized law always has a positive pressure, in contrast to the original law (1.4). It is also seen that the RSG is an extension of the IRSG law.



Figure 4. Comparison of SG and RSG laws (Zoom).

5. An illustration: patch of liquid in free fall

As discussed in the Introduction, the derivation of the RSG EoS was motivated by simulations of wave impacts, for example sloshing of liquid methane in tanks of liquefied natural gas carriers, see *e.g.* the recent review by Dias and Ghidaglia [8]. Here, the added value of this law over the usual SG EoS is illustrated for a classical benchmark in the field (see Braeunig *et al.* [3]). This 2D benchmark studies the free fall of a patch of liquid methane surrounded by gaseous methane in a closed rigid tank. The initial geometry is given in Figure 5. The code used is FLUX-IC, which is based on the inviscid Euler equation with interface capturing, see [4].



Figure 5. Initial geometry of the liquid patch surrounded by the gas.

Figure 6 shows the plot of the pressure history along the vertical symmetry axis, Oz, of the patch for the computation performed with the classical SG EoS, where negative pressures are observed. Now, using the RSG EoS described in this article, it can be seen in Figure 7 that this unphysical behavior has been corrected. For more details on these results, the reader is referred to Costes *et al.* [6] and Mrabet [11].



Figure 6. Pressure history along the vertical symmetry axis, Oz, with SG EoS.

6. Appendix: Specific entropy function for the SG EoS

The objective of this Section is to prove the expression (2.9) of the specific entropy function for the SG EoS. Considering a fluid that satisfies EoS (1.4) and property (2.8). According to Proposition 3.1, we can write:

$$T(\rho, s) = \theta(\rho) \exp\left(\frac{s - s_0}{C_V}\right), \quad \theta(\rho_0) = T_0, \qquad (6.1)$$



Figure 7. Pressure history along the vertical symmetry axis, Oz, with RSG EoS. Note that the thermodynamic pressure is obtained by adding $1 bar \approx 10^5 Pa$ to the dynamic pressure. Hence the thermodynamic pressure is positive.

so that Gibbs relation (2.4) together with (1.4) yields:

$$\theta(\rho) \exp\left(\frac{s-s_0}{C_V}\right) ds = de - \frac{(\gamma-1)\rho e - \pi_0}{\rho^2} d\rho.$$
(6.2)

Hence, introducing the function $S \equiv C_V \exp\left(\frac{s-s_0}{C_V}\right)$, it transpires that

$$dS = \frac{de}{\theta(\rho)} - \frac{(\gamma - 1)\rho e - \pi_0}{\rho^2 \theta(\rho)} d\rho.$$
(6.3)

This means that:

$$\left(\frac{\partial S}{\partial e}\right)_{\rho} = \frac{1}{\theta(\rho)}, \qquad \left(\frac{\partial S}{\partial \rho}\right)_{e} = -\frac{(\gamma - 1)\rho e - \pi_{0}}{\rho^{2}\theta(\rho)}, \qquad (6.4)$$

and using $\left(\frac{\partial^2 S}{\partial e \, \partial \rho}\right) = \left(\frac{\partial^2 S}{\partial \rho \, \partial e}\right)$, it is easily found that:

$$\theta(\rho) = T_0 \left(\frac{\rho}{\rho_0}\right)^{\gamma-1}.$$
(6.5)

Now, returning to (6.4), we have:

$$\left(\frac{\partial S}{\partial e}\right)_{\rho} = \frac{1}{T_0} \left(\frac{\rho}{\rho_0}\right)^{1-\gamma}, \qquad (6.6)$$

$$\left(\frac{\partial S}{\partial \rho}\right)_{e} = \frac{\pi_{0}}{\rho^{2} T_{0}} \left(\frac{\rho}{\rho_{0}}\right)^{1-\gamma} - \frac{(\gamma-1)e}{T_{0}\rho} \left(\frac{\rho}{\rho_{0}}\right)^{1-\gamma} . \tag{6.7}$$

Equation (6.6) immediately yields:

$$S = \frac{e}{T_0} \left(\frac{\rho}{\rho_0}\right)^{1-\gamma} + F(\rho), \qquad (6.8)$$

where F is arbitrary function. Now, due to (6.7), we find:

$$F'(\rho) = \frac{\pi_0}{\rho^2 T_0} \left(\frac{\rho}{\rho_0}\right)^{1-\gamma}, \quad F(\rho) = -\frac{\pi_0}{\gamma \rho_0 T_0} \left(\frac{\rho}{\rho_0}\right)^{-\gamma} + F_0.$$
(6.9)

Finally returning to (6.8) we can write:

$$C_V \exp\left(\frac{s-s_0}{C_V}\right) = \frac{e}{T_0} \left(\frac{\rho}{\rho_0}\right)^{1-\gamma} - \frac{\pi_0}{\gamma \rho_0 T_0} \left(\frac{\rho}{\rho_0}\right)^{-\gamma} + F_0, \qquad (6.10)$$

or in the pressure and density variables:

$$C_V \exp\left(\frac{s-s_0}{C_V}\right) = \frac{1}{(\gamma-1)T_0\rho_0} \left(\frac{\rho}{\rho_0}\right)^{-\gamma} \left[p + \frac{\pi_0}{\gamma}\right] + F_0, \qquad (6.11)$$

that is:

$$(\gamma - 1) T_0 \rho_0 C_V \left(\exp\left(\frac{s - s_0}{C_V}\right) - 1 \right) = \left(\frac{\rho}{\rho_0}\right)^{-\gamma} \left[p + \frac{\pi_0}{\gamma} \right] - \left[p_0 + \frac{\pi_0}{\gamma} \right]. \quad (6.12)$$

Hence, the following result has been demonstrated.

Proposition 6.1. The entropy specific function of a fluid that satisfies EoS (1.4) and property (2.8) is explicitly given by the relation (6.12).

Remark 6.1. In the literature (see *e.g.* Oger *et al.* [12]), the ISG EoS (2.10) can be found. Indeed, relation (6.12) is not necessary to find the ISG EoS (2.10) from the SG EoS (1.4), and it will be briefly explained how below. However, Proposition 6.1 seems to be new.

Deriving the ISG EoS from the SG EoS. According to Gibbs relation (2.4) for isentropic transformation of the fluid, we have:

$$de = \frac{p}{\rho^2} d\rho, \text{ that is } d\left(\frac{p+\pi_0}{(\gamma-1)\rho}\right) = \frac{p}{\rho^2} d\rho, \text{ or } \frac{dp}{\gamma p+\pi_0} = \frac{d\rho}{\rho}, \quad (6.13)$$

and (2.10) follows immediately.

Glossary

Abbreviation	Fully spelled out
CFD	Computational Fluid Dynamics
EoS	Equation of State
SoS	Speed of Sound
SG	Stiffened-Gas
ISG	Isentropic Stiffened-Gas
IRSG	Isentropic Regularized Stiffened-Gas
RSG	Regularized Stiffened-Gas

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