Pareto-Optimal Assignment of Thermodyamic State Equations for LES of Transcritical Reacting Flows

Pushan Sharma[a], Davy Brouzet[a], Matthias Ihme[a]
[a] Department of Mechanical Engineering, Stanford University
488 Escondido Mall, Stanford, California, USA

1 Introduction

Accurate simulations of transcritical real fluid effects are crucial for many engineering applications, such as fuel injection in diesel engines. The ideal gas (IG) equation of state (EoS), which is used in most gaseous combustion applications, cannot capture the complex thermodynamic behavior resulting in large gradients of thermodynamic quantities in the transcritical regime. Cubic equations of state, especially the Peng-Robinson (PR) approach, have been extensively used in past studies for the accurate description of thermodynamic and transport properties across the transcritical regime. However, a better accuracy with the PR equation comes at a significantly higher computational cost compared to the IG approach. When the liquid fuel spray evaporates in a diesel fuel injection (DFI) configuration, it reaches a gaseous supercritical state at which its temperature is much higher than the critical temperature. Hence, their thermodynamic and transport properties are expected to follow ideal gas behavior. Therefore, only a small fraction of the computational domain require real fluid modeling. The objective of this work is therefore to develop a cost-constrained approach to dynamically and adaptively assign the EoS, PR or IG, depending on the local thermochemical conditions in the computational domain.

Recently, a Pareto-efficient combustion (PEC) [1] framework has been developed to deal with a similar problem, where combustion chemistry models are dynamically assigned based on local cost and accuracy metrics in gas-phase reacting flows. For instance, this framework can adaptively choose between an expensive and accurate finite rate chemistry (FRC) model and a relatively less expensive and less accurate flamelet-progress variable (FPV) model depending on the local thermo-chemical state. Motivated by the PEC approach, here we develop a Pareto-optimal equation of state (POES) framework to selectively assign the necessary EoS based on thermodynamic state. We first describe the PR formulation, followed by the concept and derivation of a drift term, which is the first step of the POES framework. Then, we show some preliminary validation of the derived drift term in the context of two-dimensional (2D) spray test cases at high pressure.

2 Equations of state: Peng-Robinson and Ideal gas

The POES framework is developed in this work using the PR cubic EoS. However, it can easily be extended for any other EoS. The PR state equation can be written as:

$$p = \frac{RT}{v-b} - \frac{a}{v^2+2bv-b^2}\ , \tag{1}$$

Correspondence to: Matthias Ihme (mihme@stanford.edu)

where R is the gas constant, v is the specific volume, and the coefficients a and b are dependent on temperature and composition to account for the effects of intermolecular forces. These coefficients along with the mixing rules for evaluating thermodynamic quantities are as follows:

$$a = \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} X_\alpha X_\beta a_{\alpha\beta} \ , \tag{2a}$$

$$b = \sum_{\alpha=1}^{N_s} X_\alpha b_\alpha \ , \tag{2b}$$

where X_α is the mole fraction of species α and

$$a_{\alpha\beta} = 0.457236 \frac{(RT_{c,\alpha\beta})^2}{p_{c,\alpha\beta}} \left(1 + c_{\alpha\beta}\left(1 - \sqrt{\frac{T}{T_{c,\alpha\beta}}}\right)\right)^2 \ , \tag{3a}$$

$$b_\alpha = 0.077796 \frac{RT_{c,\alpha}}{p_{c,\alpha}} \ , \tag{3b}$$

$$c_{\alpha\beta} = 0.37464 + 1.54226\omega_{\alpha\beta} - 0.26992\omega_{\alpha\beta}^2 \ . \tag{3c}$$

The critical mixture conditions for temperature, pressure, molar volume, compressibility, and acentric factor are determined using the corresponding state principles:

$$T_{c,\alpha\beta} = \sqrt{T_{c,\alpha} T_{c,\beta}}(1 - k_{\alpha\beta}) \ , \tag{4a}$$

$$p_{c,\alpha\beta} = Z_{c,\alpha\beta} \frac{\mathcal{R} T_{c,\alpha\beta}}{v_{c,\alpha\beta}} \ , \tag{4b}$$

$$v_{c,\alpha\beta} = \frac{1}{8}\left(v_{c,\alpha}^{\frac{1}{3}} + v_{c,\beta}^{\frac{1}{3}}\right)^3 \ , \tag{4c}$$

$$Z_{c,\alpha\beta} = \frac{1}{2}\left(Z_{c,\alpha} + Z_{c,\beta}\right) \ , \tag{4d}$$

$$\omega_{\alpha\beta} = \frac{1}{2}\left(\omega_\alpha + \omega_\beta\right) \ , \tag{4e}$$

where $\mathcal{R}$ is the universal gas constant, and T_c, p_c, v_c, Z_c are the critical temperature, pressure, molar volume, and compressibility factor, respectively. $k_{\alpha\beta}$ is the binary interaction parameter, and finally, ω is the acentric factor. On the other hand, the ideal gas EoS is:

$$pv = RT \ . \tag{5}$$

3 Drift term for POES

The idea of POES is to perform a dynamic EoS assignment based on estimates of local modeling error and computational cost of using PR and IG. However, the local modeling error is not directly available during the simulation without evaluating the full thermodynamic conditions using both EoS for the whole domain, and advancing the solution in time, which defeats the purpose of cost optimization in POES. Instead, we evaluate a drift term, $\widetilde{D}_\psi$, which is a first order estimate of the rate of departure of the predicted value of a quantity of interest (QoI), ψ, when computed using IG compared to a more accurate EoS, such as the PR equation. We choose pressure, p, as the QoI to derive the drift term in POES. The

idea is schematically shown in Fig. 1. Starting from an initial condition, p_{IG} and p_{PR} corresponding to IG and PR respectively, we can write the pressure at the next time step as:

$$p_{\mathrm{IG}}(t_{n+1}) = p_{\mathrm{IG}}(t_n) + \widetilde{D}_t(p_{\mathrm{IG}}(t_n)) + \mathcal{O}(\Delta t^2)\,, \tag{6a}$$

$$p_{\mathrm{PR}}(t_{n+1}) = p_{\mathrm{PR}}(t_n) + \widetilde{D}_t(p_{\mathrm{PR}}(t_n)) + \mathcal{O}(\Delta t^2)\,. \tag{6b}$$

Subtracting these two equations, we get the conservative form for the pressure drift term (removing the tilde from all equations for clarity):

$$D_p = \underbrace{\Delta p(t_n)}_{C_{\Delta p_{\mathrm{init}}}} + \underbrace{\left[D_t\left(p\right)|_{p=p_{\mathrm{PR}}} - D_t\left(p\right)|_{p=p_{\mathrm{IG}}}\right]\Delta t}_{C_{\mathrm{drift}}}\,, \tag{7}$$

where $D_t\left(p\right)$ can be written as a function of the conservatives as the following:

$$D_t(p) = \frac{\partial p}{\partial e}\Big[D_t(\rho e_t) - uD_t(\rho u) - vD_t(\rho v)\Big] + \sum_{j=1}^{N_s-1}\frac{\partial p}{\partial Y_j}D_t(\rho Y_j)\,, \tag{8}$$

where Δt is the simulation timestep, e_t is the total energy, u and v are the two velocity components, Y_j is the j-th mass fraction and N_s is the total number of species in the system.

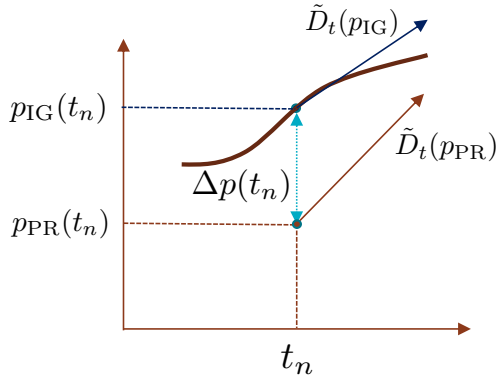

Figure 1: Schematic illustration of the drift term

3.1 Formulation of $\frac{\partial p}{\partial e}$

Following the chain rule, the derivative can be written as:

$$\frac{\partial p}{\partial e} = \frac{\partial p}{\partial T}\frac{\partial T}{\partial e}\,. \tag{9}$$

Starting from the PR EoS, we can get the derivative with respect to T as:

$$\left(\frac{\partial p}{\partial T}\right)_{v,X_i} = \frac{R}{v-b} - \frac{\left(\frac{\partial a}{\partial T}\right)_{X_i}}{v^2+2bv-b^2}\,, \tag{10a}$$

$$\left(\frac{\partial a}{\partial T}\right)_{X_i} = -\frac{1}{T}\sum_{\alpha=1}^{N_s}\sum_{\beta=1}^{N_s}X_\alpha X_\beta a_{\alpha\beta}G_{\alpha\beta}\,, \tag{10b}$$

$$G_{\alpha\beta} = \frac{c_{\alpha\beta}\sqrt{\frac{T}{T_{c,\alpha\beta}}}}{1+c_{\alpha\beta}\left(1-\sqrt{\frac{T}{T_{c,\alpha\beta}}}\right)}\,. \tag{10c}$$

On the other hand, the specific internal energy can be written as:

$$e = h^0 - RT + K_1 \left[a - T \left(\frac{\partial a}{\partial T} \right)_{X_i} \right] . \tag{11}$$

Starting from here, the partial derivatives can be obtained:

$$\frac{\partial e}{\partial T} = \frac{\partial h^0}{\partial T} - R - K_1 T \left(\frac{\partial^2 a}{\partial T^2} \right)_{X_i} , \tag{12a}$$

$$\left(\frac{\partial^2 a}{\partial T^2} \right)_{X_i} = 0.457236 \frac{R^2}{2T} \sum_{\alpha=1}^{N_s} \sum_{\beta=1}^{N_s} X_\alpha X_\beta c_{\alpha\beta} (1 + c_{\alpha\beta}) \frac{T_{c,\alpha\beta}}{p_{c,\alpha\beta}} \sqrt{\frac{T_{c,\alpha\beta}}{T}} , \tag{12b}$$

$$K_1 = \frac{1}{2\sqrt{2}b} \ln \left(\frac{v + (1 - \sqrt{2})b}{v + (1 + \sqrt{2})b} \right) . \tag{12c}$$

For the ideal gas EoS, the pressure derivative with respect to temperature is simply:

$$\left(\frac{\partial p}{\partial T} \right)_{v,X_i} = \frac{R}{v} . \tag{13}$$

The specific internal energy can be written as:

$$e = h^0 - RT , \tag{14}$$

leading to

$$\frac{\partial e}{\partial T} = \frac{\partial h^0}{\partial T} - R , \tag{15}$$

where h^0 is the specific enthalpy corresponding to ideal gas, which can be evaluated from NASA polynomials.

3.2 Formulation of $\frac{\partial p}{\partial Y_j}$

The derivative with respect to Y_j are:

$$\frac{\partial p}{\partial Y_j} = \frac{\partial R}{\partial Y_j} \frac{T}{v - b} + \frac{RT}{(v - b)^2} \frac{\partial b}{\partial Y_j} - \frac{\frac{\partial a}{\partial Y_j}}{v^2 + 2bv - b^2} + \frac{2a(v - b)}{(v^2 + 2bv - b^2)^2} \frac{\partial b}{\partial Y_j} \tag{16}$$

where

$$\frac{\partial R}{\partial Y_j} = RW \left(\frac{1}{W_j} - \frac{1}{W_{N_s}} \right) , \tag{17a}$$

$$\frac{\partial a}{\partial Y_j} = \frac{2W}{W_j} \sum_{\alpha=1}^{N_s} X_\alpha a_{\alpha j} - \frac{2W}{W_{N_s}} \sum_{\alpha=1}^{N_s} X_\alpha a_{\alpha N_s} , \tag{17b}$$

$$\frac{\partial b}{\partial Y_j} = W \left(\frac{b_j}{W_j} - \frac{b_{N_s}}{W_{N_s}} \right) , \tag{17c}$$

$$W = \frac{1}{\sum_{\alpha=1}^{N_s} \frac{Y_\alpha}{W_\alpha}} . \tag{17d}$$

4 Application to a 2D Spray

A two-dimensional spray simulation is performed for *a-priori* validation of the drift term evaluation. A fully compressible finite-volume solver [2] is used to perform the simulations. It solves the continuity, momentum, energy and species equations using a fourth-order accurate spatial discretization scheme and a 2^{nd} order ENO reconstruction scheme in regions of high pressure and density gradients. A strong stability preserving 3^{rd} order Runge-Kutta scheme is employed for time-advancement with a maximum unity CFL number. In this simulation, n-dodecane is injected in a pre-heated nitrogen environment at 1000 K and 6 MPa ambient pressure. The spray simulation is first run for about 300 μs considering the real fluid effects everywhere in the domain, and using the double-flux method to avoid spurious pressure oscillations [2]. Then, two different approaches are used to evaluate the solution for a few timesteps: (1) continuing with the PR-EoS approach and double-flux solver, and (2) with the IG-EoS without the double-flux method. With this, we can compute numerically the drift term in Eq. 7 and compare them to the theoretical formulation previously presented.

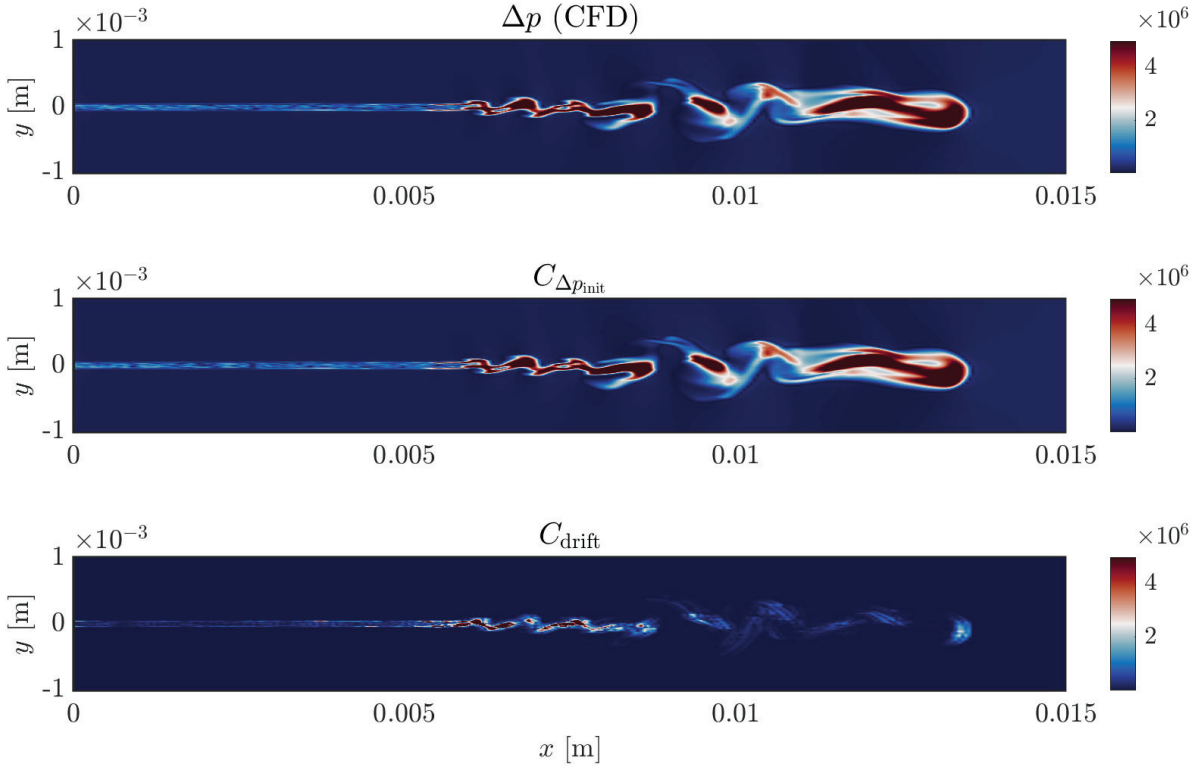

Figure 2: Difference in pressure between the solutions using the PR-EoS and IG-EoS. Top: Drift term in Eq. 7 computed numerically. Middle: First right-hand side (RHS) term in Eq. 7. Bottom: Second RHS term in Eq. 7. The units are in Pascals.

The difference in pressure between these two approaches using the simulation results is shown in Fig. 2 (top). The middle and bottom contour plots of Fig. 2 correspond to the contribution of Δp_{init} and drift term C_{drift} (see Eq. 7), respectively. The overall drift term, which is the sum of Δp_{init} and C_{drift}, coincide with the Δp numerical results, implying that the theoretical POES drift term derivation is accurate. Furthermore, the drift term with p as QoI is able to identify the regions with high fuel mass fraction (see Fig. 3), where the real fluid effects are expected to be significant. Thus, this formulation should be able to assign the correct EoS in different regions.

It is also important to note that $C_{\Delta p_{\text{init}}}$ is significantly larger than C_{drift}, which implies that a drift term

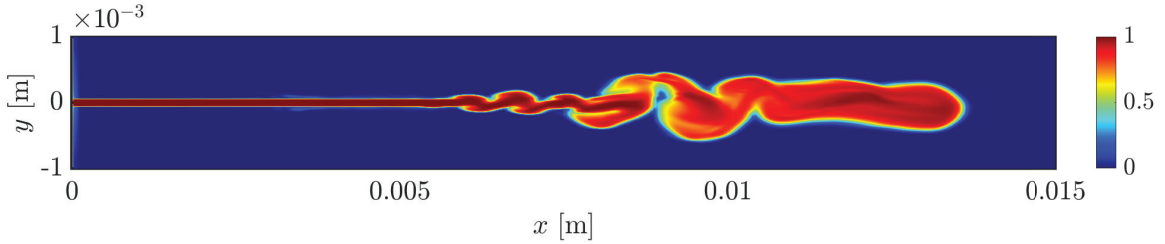

Figure 3: Fuel mass fraction.

based on only $C_{\Delta p_{\text{init}}}$ might be sufficient to assign effectively the modeling strategy. However, C_{drift} captures the temporal effects of the flow on the pressure field, which may be large for a larger time step Δt, as per Eq. 7. Further investigations are required to conclude about the relative importance of the two terms in Eq. 7.

5 Conclusions

A Pareto-optimal equation of state (POES) framework is developed for efficient utilization of different equations of state in different regions of the computational domain. The POES approach identifies the use of either the Peng-Robinson or the ideal gas equation based on the local drift-term evaluation. In this work, we choose pressure as the quantity of interest, and derive the drift-term in pressure between a PR-EoS and an IG-EoS formulation. We formulate this drift term using the conservative variables as the state vector, as the total derivatives of these quantities are usually available in numerical CFD solvers. We validate the formulation of the drift term with an *a-priori* analysis in the context of a 2D spray simulation. We show that the analytical derivation of the drift term coincides with the pressure difference between two EoS solutions computed from the simulation results. At this stage, several open questions concerning the importance of different terms in the formulation and the model assignment require further investigation and development.

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