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DYNAMICS OF GAS-LIQUID INTERFACES IN HIGH-PRESSURE SYSTEMS

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Summary This paper summarizes recent theoretical work aimed at explaining the dynamics of gas-liquid interfaces in high-pressure systems. Imaging has long shown that at certain high-pressure conditions, the presence of discrete two-phase flow processes becomes diminished. The molecular gas-liquid interface is replaced by a diffusion dominated shear-layer that evolves in the presence of exceedingly large but continuous thermo-physical gradients. Analysis reveals that the two-phase interface breaks down not necessarily because of vanishing surface tension forces, but because of thickened interfaces in a state of nonequilibrium due to the presence of thermal gradients and an inherent reduction in the molecular mean free path.

INTRODUCTION

Research over the past decade has provided significant insights into the structure and dynamics of multiphase flows at high pressures [1–4]. There are two extremes that must be considered. At subcritical, or certain supercritical operating pressures relative to the injected liquid component, the classical situation exists where a well defined molecular interface separates the injected liquid from ambient gases due to the presence of surface tension. Interactions between dynamic shear forces and surface tension promote primary atomization and secondary breakup processes that evolve from a dense state, where the liquid exists as sheets filaments or lattices intermixed with sparse pockets of gas, to a dilute state, where drop-drop interactions are negligible and dilute spray theory can be used. When operating pressures exceed the critical pressure of the injected liquid, however, the situation can become quite different. Under these conditions, internal thermal gradients can form within the gas-liquid interface due to a combination of thickening within the interface and reduced molecular mean free path. The interfacial structure enters the continuum length scale regime and disappears as interfacial fluid temperatures rise above the critical temperature of the local mixture. Lack of inter-molecular forces, coupled with broadening interfaces, promote diffusion dominated mixing prior to atomization. As a consequence, injected jets evolve in the presence of exceedingly large but continuous thermo-physical gradients in a manner markedly different from classical assumptions.

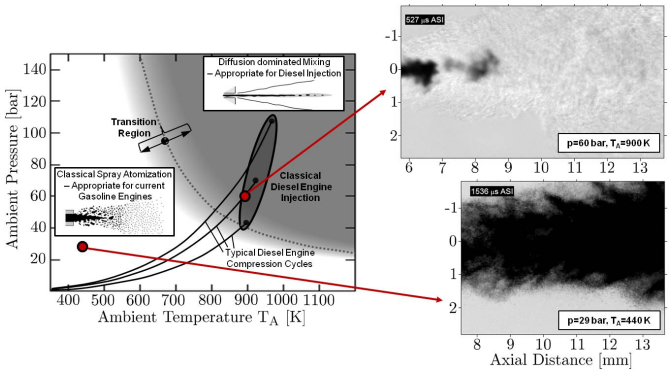

Figure 1: The regime diagram (left) describes conditions where n-dodecane injected at a temperature of 363 K into nitrogen transitions to a dense supercritical jet without drop formation. High-speed imaging of a dense supercritical jet (top right) and spray (bottom right) illustrates the change induced as a function of different ambient conditions (Images on right courtesy of L. M. Pickett, Sandia National Laboratories).

Detailed analysis suggests that the transitional changes described above are controlled by the multicomponent nature of the gas-liquid interface [5, 6]. A key output are regime diagrams for liquid injection such as the example shown in Fig. 1. This figure shows results for n-dodecane injected at a temperature of 363 K into gaseous nitrogen at varying ambient pressures and temperatures. The classical spray regime (highlighted in white) and diffusion dominated mixing regime (gray) are found using a Knudsen number criterion based on the molecular mean free path within the interface divided by the interfacial thickness (See Ref. [5]). Ambient gas pressure-temperature traces, which span a set of conditions for different Diesel engine compression cycles, are shown as follows: (a) turbo-charged (2.5 bar, 363 K), (b) medium-load (1.6 bar, 343 K), and (c) light-load (1 bar, 335 K). Fuel injection occurs at full compression conditions indicated by the three respective end points. Note that only at light-load operation does there appear to be a chance that classical fuel spray atomization takes place. These predictions have been corroborated using imaging to visualize the features of dense-fluid jets (top right image in Fig. 1) and classical spray atomization (bottom right image).

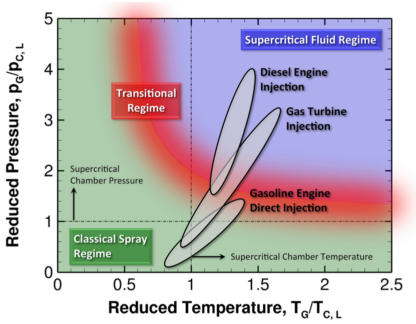

Figure 2: Typical operating envelopes in advanced Diesel, gas turbine, and gasoline direct injection systems.

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DISCUSSION

Applying the theory to a variety of system specific operating conditions suggests that almost all modern high-performance combustion devices operate over ranges of pressures and temperatures in the vicinity of, or across, the transitional regime [7, 8]. Figure 2 shows the typical operating envelopes associated with advanced Diesel, gas turbine, and gasoline direct injection systems using n-dodecane, n-decane, and iso-octane as respective fuel surrogates. The diagram is constructed for liquid injection temperatures from 300 to 363 K by normalizing the ambient gas pressure and temperature using the critical properties of the liquid phase. The Classical Spray Regime is highlighted in green, the Supercritical Fluid Regime in blue, and the Transitional Regime in red. Respective operating envelopes are indicated by the oval white areas. In each case the operational envelopes cross into the Transitional Regime, which highlights the need study these regimes simultaneously.

To further understand the dynamics of high-pressure injection, the large-eddy simulation technique has been applied using real-fluid thermodynamics and transport [9]. Liquid n-dodecane at 363 K is injected into a quiescent gaseous mixture at 900 K and 60 bar, which are precisely the same conditions represented by the medium-load compression trace shown in Fig. 1. Results from a high-resolution case (2 μm spacing across a 0.09 mm injector nozzle) are shown in Fig. 3 (see Lacaze et al. [9]). A three-dimensional rendering of the injected fuel jet is shown in the center. Fuel is injected from left to right. The red iso-surface marks the central liquid core where large density gradients exist. These gradients induce high shear forces through strongly coupled interactions between turbulence and nonideal multicomponent thermodynamics and transport processes. Instabilities form in these regions creating flow structures that entrain air and generate intense turbulence. These structures are highlighted by the yellow (500 m/s) to blue (50 m/s) iso-surfaces. Molecular diffusion completes the mixing, as shown by the more diffuse nature of the temperature field in the lower panel (363 K in dark blue to 900 K in red). Significant variations in the local speed of sound also occur. Scalar mixing within the shear-layer causes a strong decrease in the speed of sound, which reaches a minimum of approximately 200 m/s in the shear region of the jet between 30 and 70 diameters downstream, compared to 1008 m/s for the pure fuel jet at injection. The ambient speed of sound is approximately 600 m/s. The transonic variation generates pressure fluctuations of approximately ±5 bar through compression-expansion effects. These pressure variations modify local turbulent flow characteristics, which further enhance transient mixing processes.

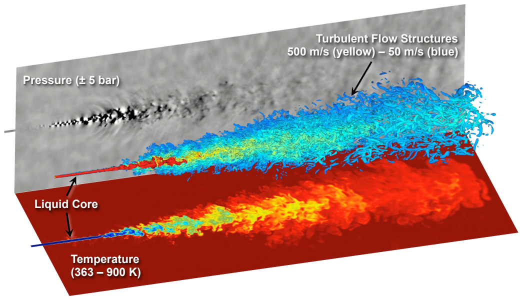

Figure 3: Three dimensional rendering liquid n-dodecane injected into nitrogen at $t = 200\ \mu$s. The red iso-surface marks where density is 200 kg/m^3, the blue iso-surface marks a Q-criterion threshold that localizes coherent turbulent structures, the bottom panel shows the temperature and rear the pressure.

CONCLUSIONS

Recent theory aimed at explaining what causes the widely observed transition from classical spray dynamics to dense-fluid mixing in multiphase systems at high pressures suggests that it occurs due to nonequilibrium processes induced through thickening of the gas-liquid interface combined with a significant reduction of the molecular mean free path. This allows formation of temperature gradients within the interface, which ultimately leads to its disintegration. The resulting shear-layer then evolves in the presence of exceedingly large but continuous thermo-physical gradients in a manner markedly different from classical assumptions. Three regimes must be considered: (1) the Classical Spray Regime, (2) the Transitional Regime, and (3) the Supercritical Regime. Applying the theory across a variety of system specific operating conditions suggests that almost all modern high-performance combustion devices operate over ranges of pressures and temperatures in the vicinity of, or across, all of these regimes. Moreover, both drops and nonideal dense fluid mixing can exist in the transitional regime, which adds significant complexities to current modeling challenges. This highlights the need to understand both classical spray and supercritical fluid phenomena simultaneously in modern devices.

References

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