Unsteady burning of n-pentane liquid droplet quiescent in high-pressure oxidizing air is investigated with emphasis placed on rigorous calculation of droplet vaporization. Fully coupled conservation equations in conjunction with global reaction kinetics for chemistry are preconditioned and time-integrated by means of a dual time-stepping technique with pertinent boundary conditions. Properties of equilibrated vapor-liquid interface are evaluated by the method of Soave-Redlich-Kwong equation of state along with consistent set of mixing rules for multi-component mixtures.

Burning of liquid fuel droplet in high-pressure oxidizing gas was numerically investigated. As a specific example, the combustion of a n-pentane fuel droplet in air was examined. In addition to aforementioned assumptions, dissolution of gas to liquid phase is allowed for gaseous nitrogen only since concentration of nitrogen at the droplet surface is much greater than those of combustion products (carbon dioxide or water). This problem simplification attends the merit of separating the pressure effects from accompanying phenomena. Initial droplet diameter is 100 μm, and initial fuel droplet and air temperatures are 300 and 1500 K, respectively, and three ambient gas pressures of 15, 30 and 50 atm were examined.
Figure 1(a) and (b) plot square of droplet diameter and heat of vaporization of liquids in terms of pressure, respectively. At all pressures, reduction of surface area is more conspicuous at early stage, however, its extent is persistently decreased thereafter as droplet surface temperature gets near its pseudo wet-bulb values. In Fig. 1(a), higher ambient pressure increasingly augments the surface regression rate, i.e., the evaporation rates, and thus curtails droplet lifetime. As was noted previously and is shown in Fig. 1(b), activation of vaporization is through increasingly reduced heat of vaporization with pressures. Higher pressures cause higher surface temperature and steeper concentration gradients at the droplet surface, and elevated level of potential for phase change and diffusion results in increase in augmentation of evaporated mass. It is worth to note that decrease in mass diffusivity also takes place along with increasing in pressure so that an adverse effect on the vaporization rate occurs. However, this effect is overwhelmed by the effect of reduction on latent heat of vaporization, and is more distinct at high pressures, thereby yields a net increase of vaporization rate.
Figure 2(a) and (b) depict evolving droplet surface temperatures and its spatial gradient at droplet surface, respectively, in terms of pressures. In the present study, radial temperature profile across the droplet surface was initialized by a linear function with large gradient. Sudden increase of surface temperature immediately after initiation is primarily due to sharper temperature gradient across the liquid/gas interface (Fig. 2(a)). Flame formed after ignition in this very short period rapidly feeds heats back to the liquids, and thus induces the temperature and concentration gradients doubly precipitous. After this sudden change at interfacial boundary, increase in surface temperature becomes gradual since the potential for gas-to-liquid thermal diffusion weakens with elevated surface temperature and percentage of energy available for phase change is thus proportionally raised. Note that transients of flame formation and vaporization are considerably altered by initial temperature profile. In Fig. 2(a), temporal evolution of surface temperatures at 50 atm (solid line) are in general accordance with previous analytical results (solid circle) except the regime of ignition and flame development (1∼2 ms). Evidently, with allowance of continuously varying initial temperatures, ignition occurs immediately after process initiation and
thus exhibits no inflection point on a temporal profile of temperature. Impulsive rise of droplet surface temperature intensified by ignition and corresponding energy release is also observed in Fig. 2(b), which depicts the temporal variation of temperature gradient at the droplet surface. All surface temperatures tend to behave in a very similar fashion up to 3 msec with minimal phase lag. Heat of vaporization, a prime controller of subcritical vaporization, is increasingly reduced with pressures, thus a time interval of steep temperature gradient is reasonably shortened with increasing in pressures (Fig. 1(a)). However, Fig. 2 reveals that this reduction is only marginal and general configuration of evolution is not greatly altered by the pressures. Following onset of flame development, energy released by gas-phase reaction is transferred to droplet, increases the surface temperature, and causes augmentation of evaporation rate. Transients of initial droplet vaporization and its extent are closely connected to ignition and flame build-up processes.