

Modelling of Hydrocarbon Fuel Droplet Heating and Evaporation: Recent Results

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ABSTRACT

The most recent developments in the modelling of heating and evaporation of hydrocarbon automotive (biodiesel, Diesel, gasoline) fuel droplets at the University of Brighton are reviewed. Analyses of hydrodynamic, kinetic and molecular dynamic models, taking and not taking into account quantum-chemical effects, are presented. New results in modelling the heating and evaporation of non-spherical (spheroidal) droplets are summarised. In contrast to the models used in most engineering applications, the effects of temperature gradient within spherical droplets were taken into account based on the analytical solution to the one-dimensional heat transfer equation, assuming that the heating process is also spherically symmetric. It was shown that this approach is particularly useful for practical applications in CFD codes. In the case of multi-component droplets we need to take into account that different components evaporate at different rates, creating concentration gradients in the liquid phase. In contrast to the models used in most previous publications, our approach was based on the analytical solution to the species diffusion equation in the liquid phase. These models were implemented into the ANSYS Fluent CFD code using User-Defined Functions (UDF). The predictions of this code with the new models were verified against the results predicted by the in-house research code. In the case of hydrocarbon fuels with large numbers of components a new multi-dimensional quasi-discrete model has been developed. In this model, the contributions of individual components are replaced with the contributions of the group of components with close transport and thermodynamic properties, called quasi-components. New approaches to modelling fuel droplet heating, evaporation and ignition, based on the method of integral manifolds, and related problems are discussed. Prospects for future research are highlighted.

KEYWORDS: Droplets, hydrocarbon fuel, heating, evaporation, ignition.

NOMENCLATURE

c specific heat capacity (J/(kg·K))
 D mass diffusivity (m²/s)
 h heat transfer coefficient (W/(m²·K)) or slow manifold (-)
 k thermal conductivity (W/(m·K))
 L latent heat of evaporation (J/kg)
 \mathcal{L} positive number (-)
 \dot{m}_d evaporation rate (kg/s)
Nu Nusselt number (-)
 P source (radiation) term in Eq. (1) (K/s)
 R distance from the droplet centre (m)
 T temperature (K)

Greek

δ film thickness (μm)
 ε species evaporation rate (-) or parameter
 κ thermal diffusivity (m²/s)
 ρ density (kg/m³)
 χ, χ_Y correction factors (-)

Subscripts

d droplet
 eff effective
 g gas
 i species

t	time (s)	l	liquid
Y	mass fraction (-)	s, w	surface, wall
		0	initial

INTRODUCTION

The modelling of droplet heating and evaporation has been extensively studied for over 100 years, and the results have been summarised in numerous papers and monographs, including [1, 2]. These studies have been stimulated by various engineering applications, including those in spray fire/combustion research [3], and much progress has been made. The aim of this paper is to summarise the results of the studies most recently presented by the author and his colleagues, and to identify areas for future research. The focus will be on recent progress in the development of the hydrodynamic and kinetic models of individual spherical hydrocarbon droplet heating and evaporation, the results obtained using these models, modelling of clouds of heated and evaporated droplets, modelling of heating and evaporation of non-spherical droplets/liquid films, modelling of droplet heating and evaporation alongside the ignition of a fuel vapour/air mixture, and related problems. The prospects for future research will be summarised at the end of the paper.

Although most of the models considered in the paper do not explicitly contain fire and combustion modelling, the processes which these models describe are integral parts of spray combustion as discussed in [1, 2]. Moreover, some of these models were applied to modelling water droplet heating and evaporation for applications in fire extinguishers [4] (key findings of [4] are summarised later in this paper). The results summarised in this paper are published in journals not widely read by the fire and explosion hazards community, e.g. International Journal of Heat and Mass Transfer.

SPHERICAL DROPLETS

In a series of our papers, published during the last 15 years and summarised in [1, 5], we described new approaches to modelling the heating and evaporation of mono- and multi-component droplets based on the analytical solutions to heat transfer and species diffusion equations inside droplets, and the combination of kinetic/molecular dynamics and hydrodynamic approaches to modelling the evaporation processes. These approaches proved to be efficient in numerous applications. In what follows in this section, we will summarise the basic ideas behind the relevant models developed by our group, and describe their most recent application to the modelling of heating and evaporation of hydrocarbon fuel droplets, and a recently developed approach to modelling the dynamics of clouds of heated and evaporating droplets.

Models

Assuming that droplet heating is spherically symmetric, e.g. the Marangoni effect is not taken into account, the transient heat conduction equation inside droplets can be written as [1]

$$\frac{\partial T}{\partial t} = \frac{\kappa}{R^2} \frac{\partial}{\partial R} \left(R^2 \frac{\partial T}{\partial R} \right) + P(t, R), \quad (1)$$

where $\kappa = k_l / (c_l \rho_l)$ is the liquid thermal diffusivity, k_l , c_l , and ρ_l are the liquid thermal conductivity, specific heat capacity, and density, respectively, R is the distance from the centre of the spherical droplet, t is time. The boundary and initial conditions for this equation, ignoring the effect of evaporation, can be presented as: $h(T_g - T_s) = k_l \frac{\partial T}{\partial R} |_{R=R_d}$, $T(t=0) = T_{d0}(R)$, where $T_s = T_s(t)$ is the droplet's surface temperature, $T_g = T_g(t)$ is the ambient gas temperature, $h = h(t)$ is the convective

heat transfer coefficient, linked with the Nusselt number Nu via the equation $Nu=2R_d h/k_g$, k_g is the gas thermal conductivity. To take into account the effect of evaporation the gas temperature T_g was replaced with the so-called effective temperature $T_{eff} = T_g + \rho_l L \frac{dR_d}{dt} / h$, where L is the latent heat of evaporation and $\frac{dR_d}{dt}$ is the rate of change of droplet radius due to evaporation.

For a short time step it was assumed that $h(t) = h = \text{const}$ with constant droplet radius and an analytical solution to this equation, subject to the above-mentioned boundary and initial conditions, was obtained [1]. This solution was generalised to the case when the changes in the droplet radii during the time step were taken into account [1].

Term $P(t, R)$ takes into account heating of droplets due to external thermal radiation. In contrast to the approach used in most commercial CFD codes, we took into account that this heating is a volumetric rather than a surface phenomenon [1].

For modelling multi-component droplet heating and evaporation, the same equations as used for mono-component droplets were applied, but these were complemented by the equations for species mass fractions ($Y_{li} \equiv Y_{li}(t, R)$) inside the droplets [1]

$$\frac{\partial Y_{li}}{\partial t} = \frac{D_l}{R^2} \frac{\partial}{\partial R} \left(R^2 \frac{\partial Y_{li}}{\partial R} \right), \quad (2)$$

where $i \geq 1$, D_l is the liquid mass diffusivity. Equation (2) was solved subject to the boundary condition $\left(\frac{\dot{m}_d}{4\pi R_d^2 \rho_l} \right) (\varepsilon_i - Y_{li}) = -D_l \frac{\partial Y_{li}}{\partial R} |_{R=R_d-0}$ and the initial condition $Y_{li}(t=0) = Y_{li0}(R)$, where $Y_{lis} = Y_{lis}(t)$ are liquid components' mass fractions at the droplet's surface, $\varepsilon_i = Y_{vis} / \sum_i Y_{vis}$ are species evaporation rates.

As in the case of the heat transfer equation, for a short time step we assumed that the droplet radius is constant and obtained an analytical solution to Eq. (2) subject to the previously mentioned boundary and initial conditions [1]. As in the case of Eq. (1), this solution was generalised to the case when the changes in the droplet radii during the time step were taken into account [1].

In all of the analytical solutions mentioned, the effects of recirculation in the moving droplets were taken into account by replacing k_l with $k_{eff} = \chi k_l$, and D_l with $D_{eff} = \chi_Y D_l$, where χ and χ_Y lie in the range between 1 (stationary droplets) and 2.72 (fast moving droplets). The models based on these approaches are known as the Effective Thermal Conductivity (ETC) and Effective Diffusivity (ED) models [1]. The above equations for the liquid phase were supplemented by equations for the gas phase, essentially based on the well-known Abramzon and Sirignano model [1].

The model based on the solution to Eq. (2) for all components is known as the Discrete Component (DC) model. A new approach to modelling heating and evaporation of multi-component droplets, suitable for the case when a large number of components is present in the droplets, was suggested by our group back in 2011. In contrast to the previously suggested models, designed for large numbers of components, the new model takes into account the diffusion of liquid species and thermal diffusion as in the classical DC model. This model was called the quasi-discrete model [1]. The main limitation of the original quasi-discrete model is that it is based on the assumption that fuels consist only of alkanes. The same model could be applied to the case when alkanes are replaced by another family of components. It cannot, however, be directly applied to the case of most realistic fuels, for which the contributions of various groups of components should be taken into account. This can be done in the generalised version of the quasi-discrete model, called the Multi-dimensional Quasi-discrete Model (MDQDM). In the latter model the principles of the quasi-discrete model are applied to all groups of components in realistic fuels (see [5] for further details).

In the models discussed so far the droplet heating and evaporation processes were modelled based on the hydrodynamic approximation where vapour at the droplet surface is assumed to be saturated and modelling of the evaporation is reduced to modelling of the diffusion of vapour from the droplet surface to the ambient gas. The limitations of this approximation have been well known since the pioneering papers and books published more than 100 years ago (see [5] and the references therein). In a series of models developed by our group, in the immediate vicinity of droplet surfaces (up to about one hundred molecular mean free paths), the vapour and ambient gas dynamics were studied based on the Boltzmann equations (kinetic region), while at larger distances the analysis was based on the hydrodynamic equations (hydrodynamic region). Mass, momentum and energy fluxes were conserved at the interface between these regions and between the kinetic region and liquid [5]. The boundary conditions at the liquid surface were inferred from the results of molecular dynamics calculations, taking and not taking into account the quantum chemical effects [5].

The models based on the analytical solutions to Eqs. (1) and (2) were incorporated into the commercial CFD software ANSYS Fluent via User Defined Functions (UDF) and verified using the predictions of in-house codes [6,7].

RESULTS

In this section, some results of the application of the models described in the previous section and published after the publication of review [5] are briefly summarised.

Our recent paper [8] was focused on the impacts of ambient conditions, including pressure, ambient temperature, effects of radiation, and fractions of ethanol in ethanol/gasoline fuel blends, on droplet heating and evaporation. Note that the effect of thermal radiation in this paper was taken into account not based on Eq. (1) but based on a simplified approach in which this effect was considered to be a surface phenomenon (in line with the approach used in most CFD codes). The Discrete Component (DC) model was used for the analysis. Both the full composition of gasoline fuel and circulation inside the droplets were taken into account using the ETC/ED model. The model was validated against relevant experimental data. The analysis focused on fuel blends with 0%, 5%, 20%, 50%, 85%, and 100% molar fractions of ethanol, and it was shown that the maximal droplet surface temperature is the largest and the droplet lifetime is the smallest for pure gasoline fuel. It was concluded that the addition of ethanol to gasoline fuel makes this fuel less volatile.

The author of [9] investigated the evolutions of droplet radii and temperatures for ethanol and gasoline fuels and their blends using a modified version of the DC model, taking into account the effect of the non-unity activity coefficient (AC). The universal quasi-chemical functional-group AC (UNIFAC) model was used in their analysis; gasoline fuel was approximated by 21 components. In contrast to previous studies, it was shown that droplet lifetimes predicted for pure gasoline are not always shorter than those predicted for ethanol/gasoline blends. They were shown to depend on the total vapour pressure of the mixture. The original DC model predicted ethanol/gasoline fuel droplet lifetimes with errors up to 5.7% compared to those predicted using the same model but with non-unity ACs obtained using the UNIFAC model.

DROPLET CLOUDS

The authors of [10] suggested a new model for heating and evaporating of a droplet cloud, based on a combination and further development of the approaches presented previously, focused on heating and evaporation of individual droplets, and the fully Lagrangian approach, describing the evolution of the number density of non-evaporating particles. The advantages of the fully Lagrangian approach compared with the conventional Lagrangian and Eulerian approaches were widely discussed in the literature [11, 12]. This model was incorporated into ANSYS Fluent. Its

functionality testing was performed using a two-phase back-step flow, ignoring the effects of droplets on the carrier phase. Only mono-sized and mono-component droplets were considered. It was shown that, due to non-homogeneous droplet number density distribution, the heat and mass transfer rates between the carrier phase and droplet clouds are different from those inferred from the analysis of trajectories of individual droplets. The temperature gradients in the flow were shown to have a significant indirect effect on the evolution of droplet number densities via the effects of these gradients on flow velocity.

NON-SPHERICAL DROPLETS

The models described so far are based on the assumption that all droplets are spherical, but this is far from the case for most droplets observed in engineering applications [13]. The simplest way to investigate the effects of droplet non-sphericity is to assume that droplets have reasonably simple shapes. In what follows, two types of shapes of non-spherical droplet will be considered: prolate or oblate spheroids and liquid film (which can be considered as a limiting case of an oblate spheroid).

Spheroids

The heat conduction equation inside a spheroidal body (non-evaporating droplet) was first (to the best of the author's knowledge) solved analytically more than 135 years ago [14]. This solution, however, turned out to be too complex for most practical applications. In most cases this problem (and the related problem of mass transfer inside the body) has been investigated based on the numerical solutions to the heat transfer (and mass diffusion) equations.

Omitting a review of background research in this area (see [5]) we focus on the model for spheroidal droplet heating and evaporation described in [15]. The authors of this paper focused on the numerical solution to the heat transfer equation in the liquid phase using the analytical solution to the transport equations in the gas phase presented in [16] as the boundary conditions. The temperature gradients at the surface of the droplets and inside them, and the changes in their shape during the heating and evaporation process, were taken into account, but the droplet shape was assumed to be close to that of a sphere. The effects of surface tension and relative droplet motion on their heating and evaporation were ignored. It was assumed that the droplet remains spheroidal, although the parameters of the spheroid were allowed to change with time due to heating and evaporation processes.

The model was applied to the analysis of n-dodecane droplet heating and evaporation under Diesel engine-like conditions. It was shown that local droplet surface temperatures could vary by more than 35 K and changes in local evaporation rates of up to 700% were observed. Droplet heating was shown to be more intense in the regions with greatest curvature. Higher evaporation at the droplet surface in these regions led to a decrease (increase) in droplet eccentricity for prolate (oblate) droplets. In all cases the droplet was shown to become more spherical at the end of the evaporation process (the eccentricity tended towards 1). The effect of droplet non-sphericity on their heating and evaporation was shown to be relatively weak for droplets with initial eccentricities between 2/3 and 1.5.

Liquid films

As mentioned earlier, for prolate droplets, a liquid film can be considered to be the limiting case. The importance of modelling hydrocarbon liquid film heating and evaporation, in connection with the analysis of the processes in internal combustion engines and other combustion processes is well known [17].

In contrast to most previously suggested models of the phenomenon (see [17] for the details), the authors of [18] took into account the presence of multiple components in the liquid film (a typical

situation for automotive hydrocarbon fuels). Both thermal and species diffusion inside the liquid film were taken into account. As in the case of the analysis of multi-component droplet heating and evaporation (see the discussion in the previous sections), the model suggested in [18] is based on the analytical solutions to the heat transfer and species diffusion equations in the liquid film. The film was assumed to be thin which allowed the authors of [18] to use the one-dimensional model in which both temperature and liquid species mass fractions depend only on the distance from the wall.

For the heat transfer equation, the Dirichlet boundary condition was used at the wall and the Robin boundary condition was used at the film surface. The Neumann boundary conditions were used at the wall, and Robin boundary conditions were used at the film surface for the species diffusion equations. The convective heat transfer coefficient was assumed to be constant and the convective mass transfer coefficient was inferred from the Chilton-Colburn analogy. The model was validated using the previously published experimental data referring to heating and evaporation of a film composed of mixtures of isooctane/3-methylpentane (3MP), and applied to the analysis of heating and evaporation of a 50%/50% mixture of heptane and hexadecane film in Diesel engine conditions.

Time evolution of the normalised film thickness in the case of evaporation of a 3MP and isooctane mixture film in typical Diesel engine conditions ($T_g = T_w = 302.25$ K, $T_0(x) = 293.15$ K, $\delta_0 = 602.72$ μm and $h = 14$ W/(m² K)) is shown in Fig. 1. Curves show the prediction of the model, while symbols show experimental data.

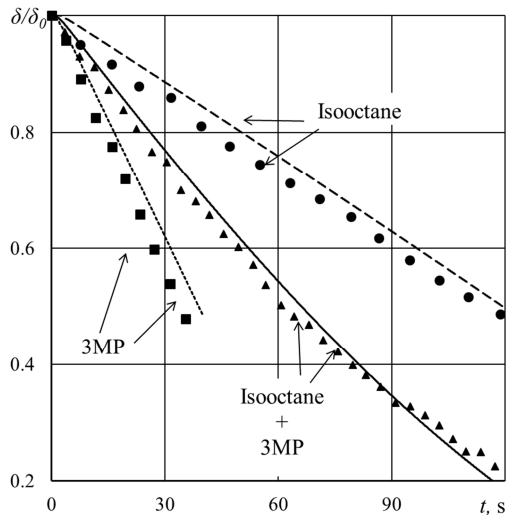


Fig. 1. Time evolution of the normalised film thickness. Circles, triangles and squares show the experimental values; solid and dashed curves show the corresponding predictions of the model. Three cases were considered: pure isooctane, pure 3MP (3-methylpentane), and a 50%/50% mixture of isooctane and 3MP. Reprinted from International Journal of Heat and Mass Transfer, Volume 117, Sazhin et al., A mathematical model for heating and evaporation of a multi-component liquid film, Pages 252–260, Copyright Elsevier (2018).

As can be seen from Fig. 1, the results predicted by the model are reasonably close to the experimental data for all three cases. This gives us confidence to apply the model to the analysis of other films including those observed for conditions relevant to combustion systems.

SPRAY HEATING, EVAPORATION AND IGNITION

The importance of modelling hydrocarbon spray heating, evaporation and ignition/combustion processes in various engineering, including automotive, applications is well recognised [19]. This modelling has been typically based on the application of computational fluid dynamics (CFD) codes [20], although the limitations of this approach have been widely discussed in the literature [1]. An alternative approach to modelling these processes can be based on the observation that they are described by systems of ordinary differential equations (ODEs) in each computational cell. These equations are commonly characterised by very large differences in the rates of change of variables. This is expected to allow the application of asymptotic methods [1]. These methods cannot replace the conventional CFD approach to the problem but can complement it by highlighting the physical background of individual processes [1]. An efficient method for the analysis of these processes was based on the theory of integral manifolds for singularly perturbed systems [21]. For autonomous systems this theory is known as the theory of invariant manifolds and is focused on the following system of equations

$$\frac{\partial x}{\partial t} = f(x, y), \quad (3)$$

$$\varepsilon \frac{\partial y}{\partial t} = g(x, y), \quad (4)$$

where $0 < \varepsilon \ll 1$, x and y are vectors in n - and m -dimensional spaces, respectively. This theory allows us to introduce a slow invariant manifold of the system to reduce its dimensions [21]. This manifold can be described explicitly, implicitly or in a parametric form [22].

A surface $y = h(x, 0)$ is called a slow manifold (surface) (zeroth approximation). The equation for this manifold can be obtained from the second equation in the above system in the limit $\varepsilon \rightarrow 0$: $g(x, y) = 0$. The first order approximation of the slow manifold can be found from the requirement

$$\frac{dg}{dt} = \frac{1}{\varepsilon} g_y g + g_x f = 0. \quad (5)$$

In most cases of the analysis of slow integral manifolds it is assumed that all functions are sufficiently smooth and therefore satisfy the Lipschitzian condition

$$\|g(x_1, y_1) - g(x_2, y_2)\| \leq \mathcal{L}(\|x_1 - x_2\| + \|y_1 - y_2\|), \quad (6)$$

where (x_1, y_1) , (x_2, y_2) are arbitrary arguments from the domain and $\mathcal{L} > 0$.

In many cases, however, these functions are non-Lipschitzian. This means that the conventional approach to system order reduction, based on the theory of integral manifolds, cannot be applied. The authors of [23, 24] showed that the order reduction of systems with non-Lipschitzian nonlinearities can be performed using a new concept of positively invariant manifolds. They discussed this concept and applied it to the analysis of spray ignition based on five ODEs (for gas temperature, fuel vapour and oxygen concentrations, droplet temperatures and droplet radii). This system was reduced to single ordinary differential equations for either the gas temperature or fuel concentration [24]. It was demonstrated that the equation for gas temperature predicts an increase in gas temperature up to the limiting value during finite time [24]. This was accompanied by the complete depletion of either fuel vapour or oxygen depending on their initial concentrations. This followed from the analysis of the equations for gas temperature and fuel concentration [24].

RELATED DEVELOPMENTS

In this section, some results of developments indirectly related to the main topic of the paper are summarised.

The authors of [25] suggested a new model for droplet drying based on the analytical solutions to the heat transfer and species diffusion equations inside spherical droplets discussed early in the paper. Small solid particles dispersed in an ambient evaporating liquid, or a non-evaporating substance dissolved in this liquid, were treated as non-evaporating components. Three key sub-processes in the process of droplet drying were taken into account: droplet heating/cooling, diffusion of the components inside the droplets, and evaporation of the volatile component. The model was applied to the drying of a spray of chitosan dissolved in water. The predicted size of the residual solid balls, after completion of the evaporation process, was consistent with those observed experimentally.

The authors of [4] presented the results of a series of experiments focused on investigation of the heating and evaporation of suspended water droplets in a hot air flow. The temperatures inside droplets were estimated based on Planar Laser-Induced Fluorescence (PLIF) imaging. Typical distributions of temperatures inside droplets at the initial stages of their heating and evaporation were presented. Also, these authors suggested a new model for heating and evaporation of a suspended droplet, taking into account temperature gradient and recirculation inside the droplet and the effect of a supporting rod. This model was based on the assumption that the heat transferred from the rod to the suspended droplet is uniformly distributed inside the droplet and its effect was considered similarly to the effect of external thermal radiation. The previously developed model for droplet heating in the presence of radiation, based on the analytical solution to Equation (1), was used. It was shown that an agreement between the model predictions and experimental data can be achieved if we take into account the reduction of the ambient gas temperature due to the presence of an evaporating droplet. Also, it was shown that the effect of the rod on droplet heating is most significant only for relatively low ambient gas temperatures (100 °C).

A new model for the puffing/micro-explosion of water-fuel emulsion droplets was suggested in [26]. The model is based on the assumption that a spherical water sub-droplet is located in the centre of a larger n-dodecane droplet. The heat conduction equation is solved inside this composite droplet using the Dirichlet boundary condition at the surface of the n-dodecane droplet. The time instant when the temperature at the interface between water and n-dodecane reaches the boiling temperature of water is identified as the start of the puffing/micro-explosion.

PROSPECTS FOR FUTURE RESEARCH

When identifying the prospects for future research the author cannot avoid being subjective and considering the specific research interests of our team. This section will be a slightly updated and shortened version of the corresponding section presented in [2]. In contrast to [2], the author will try to address not the mathematical but mainly the fire research community.

Although there has been some progress in the development of models for the heating and evaporation of non-spherical droplets, as described earlier based on [15], the model described in the latter paper is applicable only to ‘slightly’ non-spherical droplets (almost spherical). Recently, Cossali and Tonini [27] described a new approach to taking into account the effect of variable density and the diffusion coefficient on heat and mass transfer from a single component spherical droplet evaporating in an air stream. We believe that this approach is potentially suitable for the development of a model for heating and evaporation of strongly deformed spheroidal droplets. Even if this development takes place, however, a number of areas have still to be tackled. The real-life droplets are likely to be far from spheroidal. The evolution of arbitrary droplet shapes has been modelled using Level Set or Volume of Fluid (VOF) methods [28], but the use of these methods in CFD codes to model actually observed sprays would be unrealistic. Even in the case of slightly deformed spheroidal droplets the model described in [15] is not really suitable for direct implementation in CFD codes (it is based on the numerical solution to the heat conduction equation

in the liquid phase). The development of a simplified model for modelling heating and evaporation of slightly deformed droplets, similar to the ones described in [1] for spherical droplets, is still a challenge.

The models for droplet heating and evaporation described earlier are based on the assumption that a sharp interface between liquid and gas can be traced. This is valid only when this process takes place in sub-critical conditions. The generalisation of these models to supercritical conditions, when the interface between the liquid and gas phases becomes blurred, is still a major problem.

Although the methods of integral manifolds, and their applications in engineering, have been widely discussed [21-23], they are still not a commonly recognised tool of mathematical modelling for engineering. The workhorses of engineering modelling are the commercial CFD codes, in which these methods are currently not used. An attempt to combine the methods of integral manifolds with these codes was made in [29], but there have been no further developments in this direction to the best of the author's knowledge. This is an area for future research.

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