



Group contribution method for multicomponent evaporation with application to transportation fuels



Pavan B. Govindaraju^{a,b,*}, Matthias Ihme^a

^a Department of Mechanical Engineering, Stanford University, USA

^b Institute for Computational and Mathematical Engineering, Stanford University, USA

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ABSTRACT

Transportation fuels consist of a large number of species that belong to different families of compounds. Predictions of physical and chemical properties of such multicomponent fuels require the accurate description of evaporation rates of all species initially contained in the liquid phase. Existing computational approaches are yet to do this without difficulty due to the lack of experimental data for physical properties of fuel components. In addition, a vast number of assumptions, which include idealized compositions and interpolation equations calibrated using experiments, are being introduced to make the problem tractable. By addressing this issue, an approach based solely on functional groups that are present in the components of the fuel is developed. This formulation is coupled to a multicomponent evaporation model to account for non-ideal behavior of mixtures and the consideration of pressure and temperature variations. This is done by using the fuel composition to evaluate the acentric factor and critical properties of each fuel component followed by the evaluation of certain physical properties using a group contribution method. This procedure thus allows the evaluation of evaporation rates of practical fuels based only on the intrinsic functional groups and their relative abundance. Studies of common fuel blends including those belonging to the Jet-A and JP-8 classes related to evaporation rates, distillation characteristics and speciation are presented. A discussion of the effect of polar species on evaporation properties utilizing the UNIFAC approach for non-ideal mixtures is presented. Due to the generalized nature of this approach, the proposed method provides an effective alternative to existing computational techniques dedicated to multicomponent droplet evaporation.

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1. Introduction

Transportation fuels produced from refining or synthetic processes consist of a large number of species that belong to different families of organic compounds. Fig. 1 illustrates the composition of some commonly used transportation fuels in the aviation industry [1,2]. The two fuels are conventionally derived petroleum fuels which have similar lower heating values. Cycloparaffins, along with aromatics, form the majority of the fuel composition. However, physical properties of compounds from these families lack experimental data and are incompletely described [3]. Thus, the usage of detailed evaporation models is restricted by these species and demands an alternative approach. In addition, aromatic compounds are known for their roles as soot precursors and cycloparaffins dictate the energy density in fuel mixtures [4]. It is

thus important to account for detailed vaporization despite the lack of physical properties so that relevant evaporation and combustion characteristics can be captured.

Existing computational approaches introduce challenges in generalizing to realistic fuel blends due to assumptions that are introduced to describe evaporation and composition. These methods can be classified into three categories based on their approach to modeling droplet composition, namely (i) continuous thermodynamic models [5], (ii) distillation-curve methods [6] and (iii) discrete-component method. To evaluate how suitable the proposed method is in calculating multicomponent fuel evaporation characteristics, the accompanying evaporation model utilized must be very accurate. Further details regarding evaporation models for multicomponent droplets are provided in [7].

Initial approaches to the description of multicomponent droplet evaporation were dealt with using the method of continuous thermodynamics, in which the composition is represented by a continuous probability density function, usually beta, gamma or Gaussian distributions. The use of a beta distribution was justified

* Corresponding author at: Department of Mechanical Engineering, Stanford University, USA.

E-mail address: pavang@stanford.edu (P.B. Govindaraju).

Nomenclature

Greek Symbols

α	Thermal diffusivity ($\text{m}^2 \text{s}^{-1}$)
β	Recovered mass fraction
β^*	Recovered mole fraction
ϵ	Lennard–Jones potential (multiples of k_B) (K)
γ	Activity coefficient
γ^C	Combinatorial activity
γ^R	Residual activity
μ	Dynamic viscosity ($\text{kg m}^{-1} \text{s}^{-1}$)
$\nu_{i,k}$	Number of occurrences of k in species i
ω	Acentric factor
Ω_D	Collision integral
ϕ_i	Molar weighted volume fraction of species i
Ψ_{mn}	Binary interaction coefficient between species m and n
ρ	Density (kg m^{-3})
σ	Lennard–Jones radius (m)
τ	Time scale (s)
τ_d	Momentum relaxation time (s)
θ_i	Mole weighted area fraction of species i
Θ_m	Mole weighted area fraction of group m

Roman symbols

a_{mn}	Energy interaction coefficient between groups m and n
B_m	Mass Spalding number
c_l	Liquid specific heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)
c_p	Specific heat capacity at constant pressure ($\text{J kg}^{-1} \text{K}^{-1}$)
D	Diffusion coefficient ($\text{m}^2 \text{s}^{-1}$)
d	Diameter (m)
f	Evaporative correction factor
k_B	Boltzmann constant (J K^{-1})
L_v	Latent heat of vaporization (J kg^{-1})
M	Molecular weight (kg kmol^{-1})
m	Mass (kg)
M_i	Molecular weight of species i
n	Number of moles
N_c	Number of components
$N_{g,i}$	Number of groups in species i
N_g	Number of functional groups in the fuel
Nu	Nusselt number

p	Pressure (Pa)
Pr	Prandtl number
Q	Group surface area
q	Mole weighted group surface area
R	Volume contribution
r	Mole weighted volume contribution
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
T	Temperature (K)
V	Volume (m^3)
v_m	Molar volume ($\text{m}^3 \text{mol}^{-1}$)
x_i	Group mole fraction of species i
X_i	Mole fraction of species i
Y_i	Mass fraction of species i
Z	Compressibility factor
z	Co-ordination number

Subscripts

<i>air</i>	Air
<i>amb</i>	Ambient
<i>b</i>	Boiling point
<i>c</i>	Critical property
<i>d</i>	Droplet
<i>diff</i>	Diffusion
<i>eff</i>	Effective
<i>evap</i>	Evaporation
<i>f</i>	Feed
<i>g</i>	Gas
<i>l</i>	Liquid
<i>max</i>	Maximum
<i>nb</i>	Normal boiling point
<i>r</i>	Reduced
<i>s</i>	Surface
<i>sat</i>	Saturated
<i>sl</i>	Slip
<i>stp</i>	Standard temperature (298 K) and pressure (1 bar)
<i>v</i>	Vapor

in [8], which derives the distribution obeyed by relative ratios of alkanes. Further extensions of this idea were used in [9], where each family of organic compounds is assumed to obey a specific distribution. Other differences between treatments include the selection of the distribution variable (carbon number [10] instead of component molecular weight) and the model for vapor–liquid equilibrium (Raoult's law with Clausius–Clapeyron relation in favor of modified

equations of state). Transport equations for the distribution function are solved to obtain relations for properties [5].

The distillation curve model [6] is based on the fact that the Peclet number directly signifies the extent to which a zero-diffusivity model accurately predicts the evaporation rate of a droplet. This is done by interpolating a mixture property, for example, the vapor molecular weight using an exponential fit.

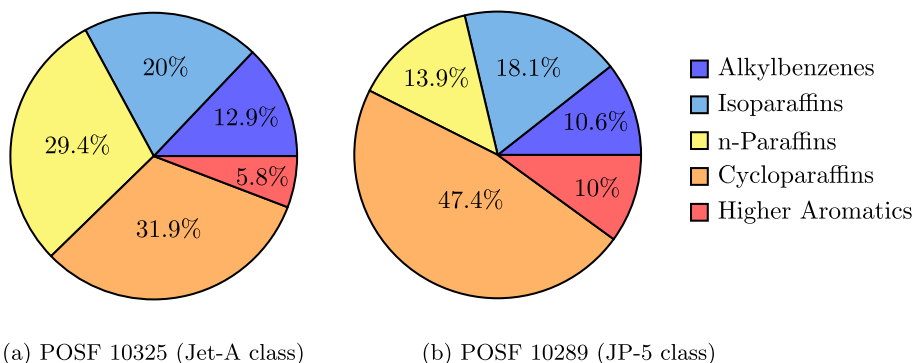


Fig. 1. Fuel composition in terms of families of organic compounds along with corresponding mass fractions for common transportation fuels (POSF 10325 and POSF 10289) used in the aviation industry.

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