# Suggested solutions TEP4170 Heat and combustion technology 8 Aug 2017

by Ivar S. Ertesvåg. Revised 10 Aug 2017, corrected 13 Feb 2018

**1)**
The sketch shows the flame height of a simple, non-premixed (diffusion) jet flame. The outflow (nozzle) velocity is gradually increased and the development of the flame is observed.
- In the first phase, the flame is laminar. Here the flame height increases with increasing velocity. This can be explained by the fact that more fuel needs a larger flame area to react since the flame is limited by the molecular diffusion. The only way to increase fuel consumption is to increase the flame.
-At a certain nozzle flow velocity, the flame becomes unstable and turbulent motion occurs. This happens when the ratio of inertia to viscous forces reaches a certain limit. The point of transition moves rapidly towards the nozzle at increasing nozzle velocity.
- In the last phase, a turbulent flame is fully developed. Here increased fuel follows more agitation (more turbulence) and leads to a larger flame area inside the flame.

**2)**
See sketch at the attached (last) page.

The flow is steady state (which means that the propagation speed of the flame equals the speed of the upstream (unburnt) flow. This is the flame speed, $u_L$.

The flame thickness $\delta_L$ can be defined as from the temperature increase, related to the temperature difference between the far upstream (unburnt) and the far downstream (burnt). The distance from a point where the temperature has increased, say, 2% of the total increase to the point where it has increased, say, 98% of the total increase.
The time scale is the ratio $\tau_c = \delta_L / u_L$

For a non-premixed flame, the velocity and length cannot be readily visualized. However, both for premixed and non-premixed flames, the time scale can be expressed from the (global) reaction rate, $\tau_c : R_{fu}^{-1}$, and the velocity and length can be expressed from the time scale and the diffusivity:
$u_L : (D / \tau_c)^{1/2}$ and $\delta_L : (\tau_c D)^{1/2}$

**3)**
The Bunsen burner is sketched in Fig. 8.3 in Turns (see last, attached page).
When a steady state flame is established and the volumetric flow rate is known, the velocity of the unburnt mixture in the tube, $v_u$ can be calculated. Alternatively, $v_u$ can be measured in the tube.

The angle $\alpha$ can be measured, and the flame speed will be the component of the unburnt velocity normal to the flame, $v_{u,n}$.

By geometrical considerations, this is expressed as $u_L (= S_L) = v_u \sin \alpha$

**4)**
Steps of soot formation and destruction in laminar diffusion (non-premixed) flames.
1. Formation of precursor species. - PAH thought to be important intermediates. Chemical kinetics plays an important role. Subject to research
2. Beginning particle formation (Particle inception). – Formation of small particles from large molecules that grows and coagulate (solidify)

3. Surface growth and agglomeration. – The small initial particles gain mass from the fuel and by agglomeration with other particles.
4. Particle oxidation. – The particles oxidate in the oxidation zone. May burn completely, or some soot particles may escape.

Typical radial temperature profile and soot concentration profile in a vertical jet of non-premixed hydrocarbon laminar flames:
Steep peak of temperature in the outer part of the jet flow (reaction zone around stoichiometric contour); steep soot peak inside this zone, falling to a low value in the high-temperature zone and outside the jet.


## 5)
chain reaction: involve the production of a radical species, which reacts to produce another radical species, and so on until formation of only stable species.
chain-initiation reaction: an elementary reaction forming one or more radical species from only stable species
chain-propagating reaction: an elementary reaction where a radical species reacts and a radical species is formed.
chain-termination reaction: an elementary reaction which consumes a radical species and forming only stable species

Radical species in the examples are O, OH, H and $HO_2$;
(CO.1) is chain-initiating; (CO.3), (CO.6) and (CO.7) are chain-propagating; none are chain terminating
Reactions (CO.2), (CO.4), and (CO.5) consume one radical species and produce two; these are called chain-branching. (In the context of the problem formulation, this can be regarded as chain propagating).


## 6)
Methane, mass: $m_{met} = 1{,}1 \text{ kg}$, molar mass: $M_{met} = 16 \text{ kg/kmol}$; amount: $n_{met} = 0{,}069 \text{ kmol}$

Overall (global) reaction:  $CH_4 + \dfrac{1}{\Phi}(2)(O_2 + \dfrac{79}{21}N_2) \rightarrow CO_2 + 2H_2O + ....$

Volume of the room: $V = 4{,}0 \cdot 4{,}0 \cdot 2{,}5 \text{ m}^3 = 40{,}0 \text{ m}^3$, temperature $T$=294 K (21 ºC),
pressure: p = 1,0 bar=100 kPa  (kPa=kN/m²=kJ/m³)
Amount of air: $n_{air} = \dfrac{pV}{R_u T} = \dfrac{100 \cdot 40{,}0}{8{,}314 \cdot 294} \text{ kmol} = 1{,}64 \text{ kmol}$

Air-fuel ratio:

actual: $\dfrac{n_{air}}{n_{met}} = \overline{AF} = \dfrac{1{,}64}{0{,}069} = 23{,}8$; stoichiometric: $\left(\dfrac{n_{air}}{n_{met}}\right)_{st} = \overline{AF}_{st} = 2 \cdot (1 + 3{,}76) = 9{,}52$

$\Phi = \dfrac{1}{\lambda} = \dfrac{\overline{AF}_{st}}{\overline{AF}} = \dfrac{9{,}52}{23{,}8} = 0{,}40$ Therefore, as $\Phi < \Phi_{min}$ (=0,50), the (well mixed) mixture is not flammable

Discussion: During the process there can be larger and smaller volumes with a flammable mixture. That is, a local $\Phi$ that is within the limits.

**7)**
Called "exact" because it is developed from the Navier-Stokes equations, just by mathematical operations, witout adding any new modelling assumptions.
Assumptions: constant density, non-fluctuating viscosity (or rather: no correlation between viscosity and velocity or pressure )

The equation for momentum reads

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j}(\tau_{ij}) + \rho f_i \quad (1)$$

Insert the Reynolds decomposition, $u_i = \bar{u}_i + u_i'$, $u_j = \bar{u}_j + u_j'$

into the equation: $\frac{\partial}{\partial t}(\rho\bar{u}_i + \rho u_i') + .... = .....$ (2)

Assume constant density and average this equation (average each term): $\frac{\partial}{\partial t}(\rho\bar{u}_i) + .... = .....$ (3)

Subtract (3) from (2): $\frac{\partial}{\partial t}(\rho u_i') + .... = .....$ (4)

Multiply (4) by $(u_i')$: $u_i'\frac{\partial}{\partial t}(\rho u_i') + .... = .....$

Make use of the relation $d(u_i'^2) = 2u_i' \cdot du_i'$: $\frac{\partial}{\partial t}(\rho\tfrac{1}{2}u_i'^2) + .... = .....$

average this equation: $\frac{\partial}{\partial t}(\rho\tfrac{1}{2}\overline{u_i'^2}) + .... = .....$   which is the equation given in the problem

Interpretation of the terms (enumerated from the left):
(1): change (increase) with time, storage
(2): carried with the mean flow (mean convection)
(3): transported with molecular motions, molecular diffusion
(4): transported with turbulent motions, turbulence diffusion
(5): production of turbulence energy due to interaction between mean-flow gradients and turbulent motions; transfer of mechanical energy from mean motion to turbulent motions
(6): degradation of kinetic energy due to molecular motions (viscous forces), "dissipation"; transfer of energy from kinetic energy to thermal energy

Terms (1), (2) (3) and (5) include only quantities that are already part of the problem (including a model for the Reynolds stresses found in Term 5) and need no further modelling. Terms (4) and (6) have to be modelled, that is, expressed from quantities found from the quantities resolved (already or with additional quantities).

**8)**
Based on the equation in Problem 7, term 4 and 5 are modeled, while term 6 found from a separate equation:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k\bar{u}_j) = \frac{\partial}{\partial x_j}(\mu\frac{\partial k}{\partial x_j}) + \frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_k}\frac{\partial k}{\partial x_j}) + \rho P_k - \rho\varepsilon$$

where

$$P_k = -\rho\overline{u_i'u_j'}\frac{\partial\bar{u}_i}{\partial x_j} = \mu_t(\frac{\partial\bar{u}_i}{\partial x_j} + \frac{\partial\bar{u}_j}{\partial x_i})\frac{\partial\bar{u}_i}{\partial x_j}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_j}(\rho\varepsilon\bar{u}_j) = \frac{\partial}{\partial x_j}(\mu\frac{\partial\varepsilon}{\partial x_j}) + \frac{\partial}{\partial x_j}(\frac{\mu_t}{\sigma_\varepsilon}\frac{\partial\varepsilon}{\partial x_j}) + \rho c_{\varepsilon 1}\frac{\varepsilon}{k}P_k - \rho c_{\varepsilon 2}\frac{\varepsilon}{k}\varepsilon$$

Here, $\sigma_k, \sigma_\varepsilon, c_{\varepsilon 1}, c_{\varepsilon 2}$ are model constants and $\mu_t$ is the (dynamic) turbulence viscosity.

**9)**
The mixing length model expresses the Reynolds stresses (essentially the shear stress in a simple boundary layer type of flow),

$$-\rho\overline{u_1' u_2'} = \mu_t \frac{\partial \overline{u_1}}{\partial x_2} = \rho l^2 \left| \frac{\partial \overline{u_1}}{\partial x_2} \right| \frac{\partial \overline{u_1}}{\partial x_2}$$

When using the $k - \varepsilon$ model, we express the turbulence viscosity as $\mu_t = \rho C_\mu \dfrac{k^2}{\varepsilon}$ and the mean velocity field (and its gradient) is resolved. Hence, all quantities are known, except the mixing length, which now can be found from $\mu_t = \rho C_\mu \dfrac{k^2}{\varepsilon} = \rho l^2 \left| \dfrac{\partial \overline{u_1}}{\partial x_2} \right|$ or $l^2 = \dfrac{\mu_t}{\rho \left| \dfrac{\partial \overline{u_1}}{\partial x_2} \right|} = \dfrac{C_\mu k^2}{\varepsilon \left| \dfrac{\partial \overline{u_1}}{\partial x_2} \right|}$

**10)**
Key words (the exam answer should be more elaborated, see details in textbook):

Two main parts: Cascade model and reactor model

The cascade model describes the transfer of kinetic energy from mean motions to larger and smaller scales of turbulence; provide a link between mean motion (described by the turbulence model) and the small eddies or fine structures (where reactions are assumed to occur)
The reactor model for the fine structures; provide the species reaction rate from a mass balance of the reactor.
The mean reaction rate is obtained from a combination of the cascade-model expressions and the reactor reaction rate.