Estimating reaction rates from models of variable-density turbulent flow

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Interfaces and Mixing in Fluids, Plasmas, Materials
KITP, UC Santa Barbara
October 23-26, 2023

Variable density turbulent flow

- Two incompressible fluids $\rho_1 < \rho_2$. Density variation due to changes in composition. ρ_2/ρ_1 may be large.
- Flow is turbulent. Use averaged equations, e.g., BHR (Besnard, Harlow, Rauenzahn [2]).
- Averaged equations contain two moments of ρ: $\overline{\rho}$ and "b"

$$\overline{\rho} = \langle \rho \rangle \tag{1}$$

$$b = -\langle \rho' v' \rangle \tag{2}$$

$$= -\left\langle \rho - \overline{\rho}, \frac{1}{\rho} - \frac{1}{\overline{\rho}} \right\rangle . \tag{3}$$

b is the "negative covariance of ρ and specific volume $v = 1/\rho$."

- σ^2 does *not* arise, except as an approximation.

Reactive flow

- Two fluids may react with each other. Or one may react with itself.
- Reaction rate frequently depends on the variance of the density [3, 9].

$$r = k \left[1 - \frac{\sigma^2}{\sigma^2_{\max} \mid \rho} \right] \tag{4}$$

- Example: inertial confinement fusion (ICF) [1, 8].

Key problems

Suppose we solve fluid equations and know b and $\overline{\rho}$.

- How do we determine the reaction rate, which requires knowledge of σ^2 (and $\overline{\rho}$)?
- What is the uncertainty in our estimate of σ^2?
- How does this uncertainty depend on the density variation, or more specifically, on the ratio ρ_2/ρ_1?

Previous efforts

- Expansions in fluctuations. E.g.,

$$b = \frac{\overline{\rho'^2}}{\overline{\rho}^2} - \frac{\overline{\rho'^3}}{\overline{\rho}^3} + \cdots + (-1)^n \frac{\overline{\rho'^n}}{\overline{\rho}^n} + (-1)^{n+1} \frac{\overline{\rho'^{n+1} v}}{\overline{\rho}^n},$$

  - Remainder frequently diverges, or converges very slowly.
  - Only useful for small $r = \rho_2/\rho_1 - 1$.
- Closure approximations [9, 7, 6]. E.g.,

$$\frac{\sigma^2}{\overline{\rho}^2} = \frac{b - (Sk)\cdot b^{3/2} + 2b^2}{(1+b)^2} + \frac{\langle \rho'^2 v'^2 \rangle}{(1+b)^2}.$$

  Then moments Sk (skewness) and $\langle \rho'^2 v'^2 \rangle$ are closed in terms of b and $\overline{\rho}$.
  - Doesn't provide uncertainty estimates.
  - Not clear that it is realizable.

Central result

Using moment methods, can obtain

- Exact bounds
$$b \cdot \frac{\overline{\rho} - \rho_1}{v_1 - \overline{v}} \leq \sigma^2 \leq b \cdot \frac{\rho_2 - \overline{\rho}}{\overline{v} - v_2}.$$
  - $\overline{v} = (b+1)/\overline{\rho}$. Also, $v_i \equiv 1/\rho_i$.
- Can evaluate dependence on $r = \rho_2/\rho_1 - 1$. Wide bounds when r is large.
- Simple closure, based on geometric mean:
$$\sigma^2 = b \cdot \sqrt{\frac{(\overline{\rho} - \rho_1)(\rho_2 - \overline{\rho})}{(v_1 - \overline{v})(\overline{v} - v_2)}}. \quad (5)$$
  Guaranteed to be realizable.

Moment methods

b can be written in many ways:

$$b = -\langle \rho' v' \rangle \tag{6}$$

$$b = \overline{\rho}\,\overline{v} - 1 \tag{7}$$

$$b = \frac{1}{\tilde{v}^2}\,\widetilde{\mathrm{var}}(v), \tag{8}$$

where the tilde denotes mass-averaging.

- We use the second expression.
- Knowing b and $\overline{\rho}$ equivalent to knowing $\overline{\rho}$ and $\overline{v}$, i.e, moments of order 1 and -1.
- Bounding σ^2 in terms of b and $\overline{\rho}$ is *equivalent* to bounding moment of order 2 in terms of moments of order 1 and -1.
- This is a generalized “Chebyshev” problem.
  - Markov (1884). Continued fractions. Moments $\mu_i = \langle x^i \rangle$, $i \geq 0$.
  - Caratheodory (1907). Convexity of “moment space.”
  - Krein, Karlin [4, 5]. Generalized to “Chebyshev” systems. Moment functions can be quite general.

Chebyshev systems

- Problem:
  - Bound $\langle u_{n+1} \rangle$ given $\langle u_i \rangle$, $1 \le i \le n$, where the u_i are *generalized moment functions*.
  - $\langle u_i \rangle \equiv \int_{[t_{\min}, t_{\max}]} u_i \, d\mu$, for some Stieltjes measure μ on $[t_{\min}, t_{\max}]$.
- $(u_1, u_2, \ldots, u_n)$ is a *Chebyshev system* if

$$U \begin{pmatrix} 1, & \ldots, & n \\ t_1, & \ldots, & t_n \end{pmatrix} = \begin{vmatrix} u_1(t_1) & u_1(t_2) & \ldots & u_1(t_n) \\ u_2(t_1) & u_2(t_2) & \ldots & u_2(t_n) \\ \vdots & \vdots & \ddots & \vdots \\ u_{n-1}(t_1) & u_{n-1}(t_2) & \ldots & u_{n-1}(t_n) \\ u_n(t_1) & u_n(t_2) & \ldots & u_n(t_n) \end{vmatrix} > 0$$

  when $t_{\min} \le t_1 < t_2 < \cdots t_n \le t_{\max}$.
  - $U = \prod_{1 \le i < j \le n} (t_j - t_i) > 0$ when $u_i = t^i$.
- To derive bounds, require that both $(u_1, u_2, \ldots, u_n)$ and $(u_1, u_2, \ldots, u_{n+1})$ are Chebyshev systems.
- Extremal values given by sums of *point measures*.

Base moment space

Figure: Blue curve is $\vec{u}(\rho) = (u_1(\rho), u_2(\rho))$, where $u_1(\rho) = \rho$ and $u_2(\rho) = 1/\rho$. The base moment space, $\mathcal{M}_2$, is the convex hull of the blue curve. The measure with mean $P = (\overline{\rho}, \overline{v})$ can be achieved through convex combinations of δ_{ρ_1} and δ_{ξ}, or δ_{η} and δ_{ρ_2}. When (u_1, u_2, u_3) is a Chebyshev system, the former minimizes, and latter maximizes, $\int u_3 d\mu$.

Full moment space

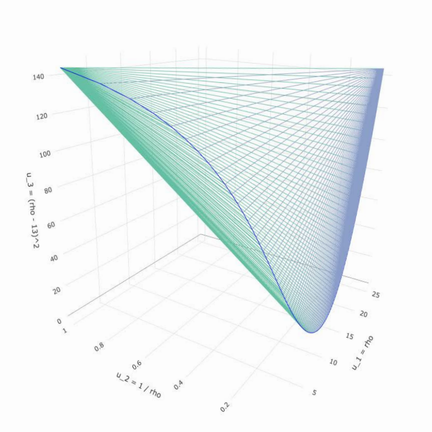

Figure: The blue curve is $\vec{u}(\rho)$, where $\vec{u} = (u_1, u_2, u_3)$, $u_1 = \rho$, $u_2 = 1/\rho$, $u_3 = (\rho - 13)^2$, $\rho_1 = 1$, and $\rho_2 = 25$. The moment space is the convex hull of the blue curve. Green lines from $\vec{u}(\rho_1)$ to $\vec{u}(\rho)$ form the lower surface of the moment space. Blue lines from $\vec{u}(\rho)$ to $\vec{u}(\rho_2)$ provide the upper boundary.

Parameters

$$r = \frac{\rho_2}{\rho_1} - 1$$

$$s = \frac{\overline{\rho} - \rho_1}{\rho_2 - \rho_1}$$

$$I_b = \frac{b}{b_{\max} \mid \overline{\rho}}$$

$$I_{\sigma^2} = \frac{\sigma^2}{\sigma^2_{\max} \mid \overline{\rho}}$$

Bounds on I_{σ^2} given I_b at $s = 1/2$.

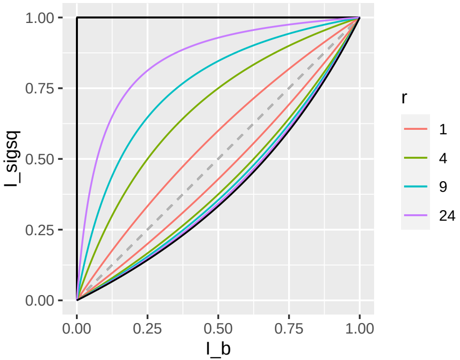

Figure: Compatibility regions for I_b and I_{σ^2}, for $r = 1, 4, 9, 24$ and $s = 1/2$. Realizable values of I_{σ^2}, given I_b, are those between the lines of the color corresponding to r.

Bounds on I_{σ^2} as function of I_b and s, for $r = 9$.

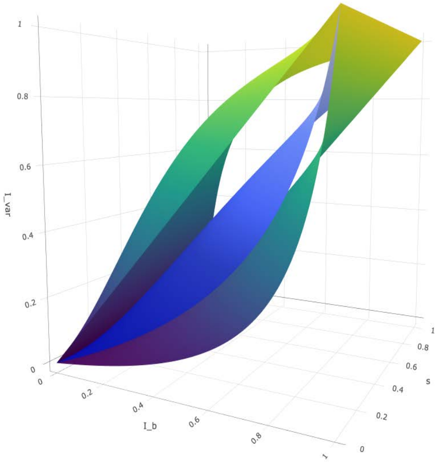

Figure: Upper and lower bounds for I_{σ^2} as a function of I_b and s. The interpolating surface, shown in blue, is given by the closure of Eq. (5).

Conclusions

- Estimating σ^2 from b and $\overline{\rho}$ was an unsolved problem.
  - Bounds were not available.
  - A closure approximation was available, but was unrealizable.
- Moment methods provide exact bounds.
- Moment methods are quite general, and may be useful in related problems.
- Bounds can also provide sanity checks for computer simulations.

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