

Stability of viscous flow. Thermodynamic point of view

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Outline

- 1 Thermodynamic system - fundamental quantities
 - Thermodynamic states
- 2 Classical mechanics of mechanical systems
 - Conservation Laws
 - Canonical form of conservation laws-Poisson brackets
 - Thermodynamic systems beyond equilibrium
- 3 Variational formulation of Continuum Mechanics
 - Necessary condition for extremum
 - Balance of energy for irreversible processes
- 4 Basic assumption of continuum thermodynamics
 - Closing of the phenomenological theory
 - Thermodynamic Inequality-Constitutive equations
 - Maximum probability of state-Thermodynamic stability
- 5 Application to fluid flow stability



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*An open and growing system evolves
and it is stable. A closed system goes
to equilibrium, biologically is dead.*

Thermodynamic systems

Thermodynamics is now taken as the science based on the accepted common principles of transformations of energy and matter.

(Dialectics of MATTER and PHYSICAL FIELD)

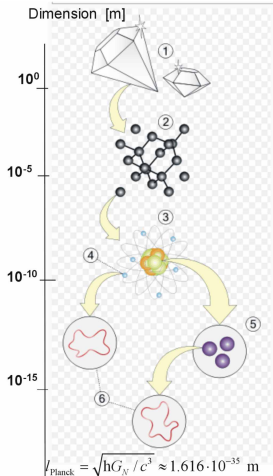
Thermodynamics is applied to investigation of real bodies - thermodynamic systems - which are composed from a great amount of interacting subsystems, e.g., atoms, molecules, cells, etc.

The examples can be: solid body, fluids, biological or ecological systems, etc.

Interaction is in thermodynamics defined like all known ways of actions of natural forces and processes.

Especially, all kinds of exchanges of energies, momentum and matters.

Geometric Dimensions of Thermodynamic Systems



Levels of magnification:

1. Macroscopic level – Matter
2. Molecular level
3. Atomic level - Protons, neutrons, and electrons
4. Subatomic level – Electron
5. Subatomic level – Quarks
6. String level

Three Generations of Matter (Fermions)

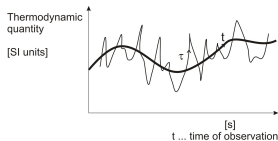
	I	II	III	
mass	3 MeV	1.24 GeV	172.5 GeV	0
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
name	up	charm	top	photon
	u	c	t	γ
	$\frac{6}{3}$ MeV	95 MeV	4.2 GeV	0
	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
Quarks	down	strange	bottom	gluon
	d	s	b	g
	<2 eV	<0.19 MeV	<18.2 MeV	90.2 GeV
	0	0	0	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
neutrino	electron neutrino	muon neutrino	tau neutrino	weak force
	ν_e	ν_μ	ν_τ	Z
	0.511 MeV	106 MeV	1.78 GeV	80.4 GeV
	-1	-1	-1	1
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
Leptons	electron	muon	tau	weak force
	e	μ	τ	W

Bosons (Forces)

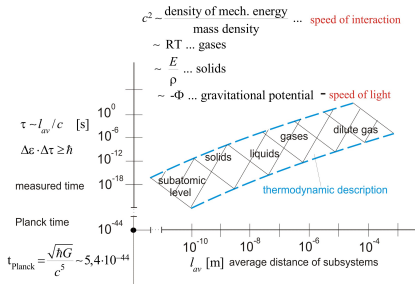
Standard_Model_of_Elementary_Particles.svg (SVG file, nominally 600 × 650 pixels, file size: 26 KB)



Time Relations in Thermodynamic Systems



t ... time of fluctuation - mean interaction time
 for macroscopic (thermodynamic) description is needed $\mathbf{dt} \ll \mathbf{dt}$



METHODS OF STATISTICAL MECHANICS AND THERMODYNAMICS

Methods of statistical mechanics and thermodynamics

System description		
	Micro	Macro- Phenomenological
Mechanics of N material particles	Dynamic variables $\dot{x}_i = \frac{\partial H}{\partial p_i}, \dot{p}_i = -\frac{\partial H}{\partial x_i} \quad (i = 1, 2, \dots, N)$ function of initial conditions and time	Macroscopic variables $f, T, \rho, u, \mathbf{u}, \mathbf{v}, \underline{\mathbf{e}}, \underline{\mathbf{t}}, \dots$ function of position \mathbf{x} and time t
	Total energy (Hamiltonian) $H(x_1, \dots, x_N, p_1, \dots, p_N)$	Balance laws of mass, momentum, moment of momentum, energy
Statistical mechanics	Partition function $\mathcal{F}(x_1, \dots, x_N, p_1, \dots, p_N)$ Liouville's equation $\mathcal{F} = 0$ Master equations (BBGKY - hierarchy, Boltzmann equation, etc.)	Dissipative processes Entropy $s = s(u, \mathbf{e}), s = s(u, \rho)$ Entropy production density $\sigma(s) = \sum_{\alpha} J_{\alpha} X_{\alpha}$
	Assumption of the most probable state $\mathcal{F}(H) = \text{const}$	Eqs of states Assumption of the state with the entropy maximum $d^2S < 0, \sigma(s) = 0$



Properties of thermodynamic systems

Probability of the fluctuation of thermodynamic parameters is related to the total entropy change and is given by the Einstein's formula

$$\text{Pr} \sim e^{\Delta S/k}$$

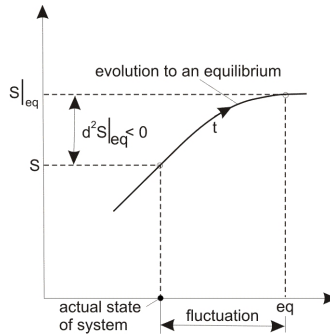
$$S_{eq} = k \ln \Gamma_{eq}$$

$$S = k \ln \Gamma$$

$$\text{Pr} = \frac{\Gamma}{\Gamma_{eq}}$$

$$\text{Pr} \sim \exp \frac{\Delta S}{k} = \exp \frac{d^2 S|_{eq}}{k}$$

PROPERTIES OF THERMODYNAMIC STATES



Entropy decrease $dS = d^2S|_{eq}$ in the surroundings of thermodynamic equilibrium $S|_{eq}$ is caused by the fluctuations of thermodynamic parameters around their equilibrium value



Properties of thermodynamic states

The all irreversible transport processes enhance the entropy

-II. Law of Thermodynamics

$$T dS|_{ir} = TdS - dQ = TdS - dU - dW \geq 0$$

Definition of entropy in classical thermodynamics

$$T dS|_{eq} = dU + dW, \quad \text{resp.} \quad T d\dot{S}|_{eq} = \dot{U} + \dot{W}$$

-systems are in equilibrium (no irreversible transport processes take place in)
Thermodynamic condition of stability of classical thermodynamics

$$dU + dW - T\Delta S > 0.$$

In equilibrium state the system reaches the maximum entropy; **only the deviations from equilibrium state (fluctuations) can the entropy decrease**

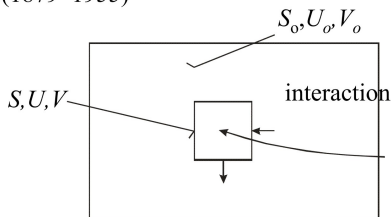
$$S - S|_{eq} = \Delta S = dS|_{eq} + \frac{1}{2} d^2 S|_{eq} + \dots$$

The measure of stability in classical thermodynamics is

$$d^2 S|_{eq} < 0$$

Probability of fluctuations

A. Einstein – 1910
 (1879–1955)



Fluctuations from equilibrium

$$-W' = T\Delta S - \Delta U - \Delta W$$

Probability of fluctuations

$$w \sim e^{-\frac{W'}{kT}} \left(= e^{-\frac{d^2S}{k}} \right)$$

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The principle of *Least Action*

The principle of *Least Action* or *Hamilton's principle*

For interacting many body system

$$\begin{aligned}\delta S &= \delta \int_{t_0}^{t_1} L(\mathbf{x}_k, \dot{\mathbf{x}}_k, t) dt = \\ &= \sum_{k=1}^N \left\{ \int_{t_0}^{t_1} \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\mathbf{x}}_k} \right) - \frac{\partial L}{\partial \mathbf{x}_k} \right) \delta \mathbf{x}_k dt + \frac{\partial L}{\partial \dot{\mathbf{x}}_k} \delta \mathbf{x}_k \Big|_{t_0}^{t_1} \right\} = 0\end{aligned}$$

with Lagrange function

$$L(\mathbf{x}_k, \dot{\mathbf{x}}_k, t) = \sum_{k=1}^N \frac{m_k \dot{\mathbf{x}}_k^2}{2} - \frac{1}{2} \sum_{k,n=1}^N V_{k,n}(|\mathbf{x}_k - \mathbf{x}_n|, t)$$

momentum is defined by

$$\mathbf{p}_k = \frac{\partial L}{\partial \dot{\mathbf{x}}_k}$$

Hamilton's principle and Hamilton - Jacobi equation

$$\mathcal{H}(\mathbf{x}_k, \mathbf{p}_k, t) = \sum_{k=1}^N \mathbf{p}_k \dot{\mathbf{x}}_k - L(\mathbf{x}_k, \dot{\mathbf{x}}_k, t)$$

Total differential of Hamilton function = energy of the system

$$d\mathcal{H}(\mathbf{x}_k, \mathbf{p}_k, t) = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} d\mathbf{p}_k + \frac{\partial \mathcal{H}}{\partial \mathbf{x}_k} d\mathbf{x}_k + \frac{\partial \mathcal{H}}{\partial t} dt = \dot{\mathbf{x}}_k d\mathbf{p}_k - \dot{\mathbf{p}}_k d\mathbf{x}_k - \frac{\partial L}{\partial t} dt$$

The **Hamilton's Equations** or so called **canonical equations** follows

$$\dot{\mathbf{x}}_k = \frac{\partial \mathcal{H}}{\partial \mathbf{p}_k}, \quad \dot{\mathbf{p}}_k = \frac{\partial \mathcal{H}}{\partial \mathbf{x}_k}, \quad \frac{\partial \mathcal{H}}{\partial t} = -\frac{\partial L}{\partial t}$$

Hamilton - Jacobi equation

$$\frac{\partial S(\mathbf{x}_k, t)}{\partial t} + \mathcal{H}\left(\mathbf{x}_k, \frac{\partial S}{\partial \mathbf{x}_k}, t\right) = 0.$$

Conservation Laws

All conservation laws follow from Lagrangian $L(\mathbf{x}_k, \dot{\mathbf{x}}_k, t)$

Balance of mass

$$\frac{dL}{dm} = \frac{\partial L}{\partial \mathbf{x}_k} \frac{d\mathbf{x}_k}{dm} + \frac{\partial L}{\partial \dot{\mathbf{x}}_k} \frac{d\dot{\mathbf{x}}_k}{dm} = \underbrace{\dot{\mathbf{p}}_k}_{=0} \frac{d\mathbf{x}_k}{dm} + \underbrace{\mathbf{p}_k}_{=0} \frac{d\dot{\mathbf{x}}_k}{dm} = 0.$$

Balance of energy... homogeneity of time

$$\frac{dL}{dt} = \frac{\partial L}{\partial \mathbf{x}_k} \dot{\mathbf{x}}_k + \frac{\partial L}{\partial \dot{\mathbf{x}}_k} \ddot{\mathbf{x}}_k + \frac{\partial L}{\partial t} = \frac{d}{dt} \left(\dot{\mathbf{x}}_k \frac{\partial L}{\partial \dot{\mathbf{x}}_k} \right) + \frac{\partial L}{\partial t},$$

or

$$-\frac{\partial L}{\partial t} = \frac{d}{dt} \left(\underbrace{\dot{\mathbf{x}}_k \frac{\partial L}{\partial \dot{\mathbf{x}}_k} - L}_{\mathcal{H}(\mathbf{x}_k, \mathbf{p}_k)} \right)$$

for $\frac{\partial L}{\partial t} = 0$, then $\mathcal{H}(\mathbf{x}_k, \mathbf{p}_k,) = \text{const}$ for isolated system

Conservation Laws

Balance of momentum. ... homogeneity of space-invariance with respect to translations

$$\delta L = \sum_{k=1}^N \underbrace{\frac{\partial L}{\partial \mathbf{x}_k}}_{\text{external forces}} \delta \mathbf{x}_k = \sum_{k=1}^N \underbrace{\dot{\mathbf{p}}_k}_{\text{inertia}} \delta \mathbf{x}_k = 0.$$

$$\sum_{k=1}^N (\dot{\mathbf{p}}_k - \mathbf{F}_k) \delta \mathbf{x}_k = 0. \dots \text{balance of forces}$$

Conservation Laws

Balance of angular momentum-moment of momentum

... isotropy of space - invariance with respect to angle of rotation θ

$$\delta \mathbf{x}_k = \delta \theta \times \mathbf{r}_k, \quad (\dot{x}_k^i = Q_j^i x_k^j)$$

$$\delta \dot{\mathbf{x}}_k = \delta \theta \times \mathbf{v}_k, \quad (\mathbf{v}_k = \dot{\mathbf{r}}_k)$$

$$\delta L = \frac{\partial L}{\partial \mathbf{x}_k} \delta \mathbf{x}_k + \frac{\partial L}{\partial \dot{\mathbf{x}}_k} \delta \dot{\mathbf{x}}_k = \dot{\mathbf{p}}_k (\delta \theta \times \mathbf{v}_k) + \mathbf{p}_k (\delta \theta \times \mathbf{v}_k)$$

$$= \delta \theta \frac{d}{dt} \left(\underbrace{\mathbf{r}_k \times \mathbf{p}_k}_{\mathbf{M}_k} \right) = 0, \quad \mathbf{M} = \sum_{k=1}^N \mathbf{M}_k \text{ const. for isolated system}$$

in the case of intrinsic angular momentum $\dot{\mathbf{M}} = \mathbf{r}_0 \times \mathbf{P}$

$$\mathbf{M} = \sum_{k=1}^N \mathbf{M}_k + \dot{\mathbf{M}}$$

In the case of external forces \mathbf{F}_k is $\sum (\mathbf{M}_k - \mathbf{r}_0 \times \mathbf{F}_k) = 0.$



Integral of motion

Those functions $\mathcal{I}(\mathbf{x}_k, \mathbf{p}_k, t)$ (functionals) of the dynamical variables $\mathbf{x}_k, \mathbf{p}_k$, which remain constant during the motion of the system are called **integral of motion**

$$\frac{d\mathcal{I}}{dt} = \frac{\partial \mathcal{I}}{\partial t} + \sum_{k=1}^N \left(\frac{\partial \mathcal{I}}{\partial \mathbf{x}_k} \dot{\mathbf{x}}_k + \frac{\partial \mathcal{I}}{\partial \mathbf{p}_k} \dot{\mathbf{p}}_k \right) = \frac{\partial \mathcal{I}}{\partial t} + \{\mathcal{H}, \mathcal{I}\}$$

Poisson bracket $\{\mathcal{H}, \mathcal{I}\}$ of the functions \mathcal{H} and \mathcal{I} is

$$\{\mathcal{H}, \mathcal{I}\} = \sum_{k=1}^N \left(\frac{\partial \mathcal{H}}{\partial \mathbf{p}_k} \frac{\partial \mathcal{I}}{\partial \mathbf{x}_k} - \frac{\partial \mathcal{H}}{\partial \mathbf{x}_k} \frac{\partial \mathcal{I}}{\partial \mathbf{p}_k} \right)$$

If the integral of the motion is not depend on the time, then

$$\{\mathcal{H}, \mathcal{I}\} = 0.$$

Beyond equilibrium thermodynamics

General time-evolution equations for beyond equilibrium systems

So called **GENERIC** formulation (General Equation for Non/Equilibrium Reversible Irreversible Coupling) [H. CH. Ottinger: Beyond Equilibrium Thermodynamics, Wiley, 2005]

$$\text{State vector } \mathbf{a} = (\rho(\mathbf{x}, t), \underbrace{\mathbf{m}(\mathbf{x}, t)}_{\rho \mathbf{v}}, \underbrace{\epsilon(\mathbf{x}, t)}_{\rho u})$$

$$\dot{\mathbf{a}} = \frac{d\mathbf{a}}{dt} = \underbrace{L(\mathbf{a}) \frac{\delta E(\mathbf{a})}{\delta \mathbf{a}}}_{\text{reversible}} + \underbrace{M(\mathbf{a}) \frac{\delta S(\mathbf{a})}{\delta \mathbf{a}}}_{\text{irreversible}} = \underbrace{\{\mathbf{a}, E\}}_{\text{Poisson bracket}} + \underbrace{[\mathbf{a}, S]}_{\text{dissipative bracket}}$$

$$E(\mathbf{a}) = \int_V \left(\frac{\mathbf{m}^2}{2\rho} + u \right) dv, \dots \text{ energy} \quad S(\mathbf{a}) = \int_V s(\rho, u) dv, \dots \text{ entropy}$$

Beyond equilibrium thermodynamics

Antisymmetric matrix describes reversible processes

$$L(\mathbf{x}, t) = - \begin{pmatrix} 0 & \frac{\partial}{\partial \mathbf{x}} \rho & 0 \\ \rho \frac{\partial}{\partial \mathbf{x}} & \left[\frac{\partial}{\partial \mathbf{x}} \mathbf{m} + \mathbf{m} \frac{\partial}{\partial \mathbf{x}} \right] & \epsilon \frac{\partial}{\partial \mathbf{x}} + \frac{\partial}{\partial \mathbf{x}} p \\ 0 & \frac{\partial}{\partial \mathbf{x}} \epsilon + p \frac{\partial}{\partial \mathbf{x}} & 0 \end{pmatrix}$$

Symmetric matrix describes time irreversible processes (dissipation)

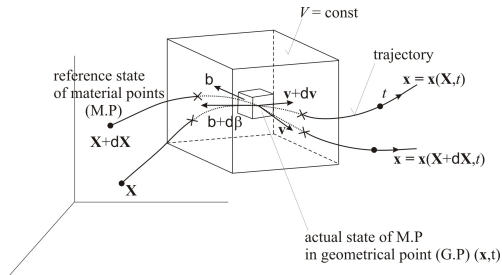
$$M(\mathbf{x}, t) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & M_{22} & M_{23} \\ 0 & M_{32} & M_{33} \end{pmatrix}$$

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Integral description

Variational principle of continuum mechanics



Local field quantities at geometrical point (\mathbf{x}, t)

$\mathbf{v}(\mathbf{x}, t)$... velocity of M.P

$\beta(\mathbf{x}, t)$... interaction velocity of surrounding with M.P.

Initial M.P. position \mathbf{X}

Action in continuum mechanics

Action functional

$$\begin{aligned} S(\mathbf{v}, \beta, \mathbf{X}) &= \int_{t_0}^{t_1} \int_V \rho \left[\frac{\mathbf{v}^2(\mathbf{x}, t)}{2} - \phi(\mathbf{x}) - u(\rho(\mathbf{X}), \mathbf{s}(\mathbf{X}, t)) - \mathbf{x}(\mathbf{X}, t)\beta(\mathbf{x}, t) \right] dv dt \\ &= \int_{t_0}^{t_1} \int_V \rho l(\mathbf{v}(\mathbf{x}, t), \beta(\mathbf{x}, t), \mathbf{X}) dv dt \end{aligned}$$

[Seliger, Whitham, Proc. Roy. Soc. A. 305, 1968]

Independent quantities (variables) $\mathbf{v}(\mathbf{x}, t)$, $\beta(\mathbf{x}, t)$, \mathbf{X}

$l(\mathbf{v}(\mathbf{x}, t), \beta(\mathbf{x}, t), \mathbf{X})$... specific lagrangian

$\frac{\mathbf{v}^2}{2}$... kinetic energy of G.P.

ϕ ... potential energy

$\mathbf{x} \cdot \dot{\beta} = x^I \dot{\beta}_I$... energy of interaction with surroundings

$u(\rho(\mathbf{X}), \mathbf{s}(\mathbf{X}, t))$... internal energy of M.P.

Motion of material point

We consider:

- the existence of the trajectory of M.P $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$,
deformation gradient

$$\frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{F} \quad \left(\frac{\partial x^i}{\partial X^I} = F^i_I \right), \quad \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \mathbf{F}^{-1} \quad \left(\frac{\partial X^I}{\partial x^i} = F^{-I}_i \right)$$
$$j = \det |\mathbf{F}|$$

- balance of mass of M.P

$$\rho(\mathbf{X}, \mathbf{F}^{-1}) = \rho_o(\mathbf{X}) \cdot j^{-1}(\mathbf{F}^{-1})$$



Motion of material point

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$$\frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{F} \quad \left(\frac{\partial x^i}{\partial X^I} = F^i_I \right), \quad \frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \mathbf{F}^{-1} \quad \left(\frac{\partial X^I}{\partial x^i} = F^{-I}_i \right)$$
$$j = \det |\mathbf{F}|$$

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Variations of functional-extremum conditions

$$\delta \left(v^2/2 \right) = v_i \delta v^i$$

$$\begin{aligned} \delta \left(\mathbf{x} \dot{\beta} \right) &= \dot{\beta} \mathbf{F} \delta \mathbf{X} + \mathbf{x} \overline{\delta \dot{\beta}_l} = \dot{\beta} \mathbf{F} \delta \mathbf{X} + x^l \left[\frac{\partial \delta \beta_l}{\partial t} + \delta \left(v^m \frac{\partial \beta_l}{\partial x^m} \right) \right] = \\ &= \dot{\beta} \mathbf{F} \delta \mathbf{X} + x^l \frac{\partial \delta \beta_l}{\partial t} + x^l \frac{\partial \beta_l}{\partial x^n} \delta v^n + x^l v^n \frac{\partial \delta \beta_l}{\partial x^n} \end{aligned}$$

$$\delta \phi = \frac{\partial \phi}{\partial x^i} \frac{\partial x^i}{\partial X^l} \delta X^l$$

$$\delta \rho = \frac{\partial \rho}{\partial X^l} \delta X^l + \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^i} \right)} \frac{\partial \delta X^l}{\partial x^i}$$

$$\delta s = \frac{\partial s}{\partial X^l} \delta X^l$$

$$\delta u = T \delta s + \frac{\rho}{\rho^2} \delta \rho \quad \dots \text{ for fluids}$$

$$= T \delta s + \frac{t_{el}^{ij}}{\rho} \delta \left[\frac{\partial X^l}{\partial x^i} \frac{\partial X^j}{\partial x^j} E_{lj}(\mathbf{X}, \mathbf{t}) \right] \quad \dots \text{ for solids}$$

Necessary condition for extremum

At condition for local extremum of functional

$$S = S(\mathbf{v}, \beta, \mathbf{X}) = \int_{t_0}^{t_1} \int_V \rho l dv dt$$

$$\text{for } l(\mathbf{x}, \mathbf{X}, t) = \frac{\mathbf{v}^2}{2} - \phi(\mathbf{x}) - u(\mathbf{X}, t) - \mathbf{x}(\mathbf{X}, t) \dot{\beta}(\mathbf{x}, t)$$

The necessary condition for local extremum (minimum)
is

$$\delta S = \int_{t_0}^{t_1} \int_V (l \delta \rho + \rho \delta l) dv dt = 0$$



Conditions derivation

$$\begin{aligned}
 \rho \delta l &= \rho \left(v_i - x^l \frac{\partial \beta_l}{\partial x^i} \right) \delta v^i - \left[\rho \left(\dot{\beta}_l + \frac{\partial \phi}{\partial x^l} \right) \frac{\partial x^l}{\partial X^l} + \rho \frac{\partial s}{\partial X^l} + \frac{\rho}{\rho} \frac{\partial \rho}{\partial X^l} \right] \delta X^l + \\
 &+ x^l \left[\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v^k)}{\partial x^k} \right] \delta \beta_l + \rho \left[\frac{\partial x^l(\mathbf{X}, t)}{\partial t} \Big|_{\mathbf{x}=\text{const}} + v^k \frac{\partial x^l}{\partial x^k} \right] \delta \beta_l + \\
 &+ \frac{\partial}{\partial x^i} \left(\frac{\rho}{\rho} \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^i} \right)} \right) \delta X^l - \left[\frac{\partial}{\partial t} (\rho x^l \delta \beta_l) + \frac{\partial}{\partial x^k} (\rho v^k x^l \delta \beta_l) \right] - \frac{\partial}{\partial x^l} \left(\frac{\rho}{\rho} \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^l} \right)} \delta X^l \right) \\
 l \delta \rho &= \left\{ l \frac{\partial \rho}{\partial X^l} - \frac{\partial}{\partial x^i} \left(l \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^i} \right)} \right) \right\} \delta X^l + \frac{\partial}{\partial x^i} \left(l \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^i} \right)} \delta X^l \right)
 \end{aligned}$$

Application of zero variation on the boundary

Under the conditions:

- balance of mass $\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v^l)}{\partial x^l} = 0$, for $\mathbf{x} \in V \times \langle t_0, t_1 \rangle$
- on the boundary $\partial(V \times \langle t_0, t \rangle)$ we consider $\delta \mathbf{v} = \delta \beta = \delta \mathbf{X} = 0$, i.e.:

$$\int_V \rho x^l \delta \beta_l \Big|_{t_0}^{t_1} dv = 0, \quad \int_{t_0}^{t_1} \int_V \rho v^k x^l \delta \beta_l da_k = 0$$

$$\int_{t_0}^{t_1} \int_{\partial V} \left(1 + \frac{p}{\rho} \right) \frac{\partial \rho}{\partial \left(\frac{\partial X^l}{\partial x^l} \right)} \delta X^l da_i = 0$$

Final form of extremum conditions

In the fixed volume V $\mathbf{x} < t_0, t_1 >$ the condition for a local extremum of the action functional has the final form

For independent variation (fluctuation) of

δv^i : $v_i = -x^l \frac{\partial \beta_l}{\partial x^i}$... velocity field for dissipative process,

$\delta \beta_l$: $\left. \frac{\partial x^i(\mathbf{x}, t)}{\partial t} \right|_{\mathbf{x}=\text{const}} = -v^i(\mathbf{x}, t)$... material point velocity
 (condition of fixed position in geometrical point $\mathbf{x} = \text{const}$),

$$\delta X^l: -\rho \left(\dot{\beta}_l \frac{\partial x^l}{\partial X^l} + \frac{\partial \phi}{\partial X^l} + \frac{\partial s}{\partial X^l} \right) + \left(1 - \frac{p}{\rho} \right) \frac{\partial \rho}{\partial X^l} - \frac{\partial}{\partial x^l} \left[\left(1 - \frac{p}{\rho} \right) \frac{\partial \rho}{\partial \left(\frac{\partial x^l}{\partial X^l} \right)} \right] = 0,$$

$$1 - \frac{p}{\rho} = - \left(h_c + x^l \frac{\partial \beta_l}{\partial t} \right) = 0,$$

$$h_c = \frac{v^2}{2} + u + \frac{p}{\rho} + \phi \dots \text{specific total enthalpy for dissipative process} \left[\frac{J}{kg} \right]$$



Integral of motion for irreversible processes

Final form of action integral

$$\begin{aligned} S &= \int_{t_0}^{t_1} \int_V \rho l dv dt = - \int_{t_0}^{t_1} \int_V \left[\underbrace{\rho \left(h_c + x^l \frac{\partial \beta_l}{\partial t} \right)}_0 + p \right] dv dt \\ &= \int_{t_0}^{t_1} \int_V p(\rho, s) dv dt \quad \dots \text{Bateman principle} \end{aligned}$$

Balance of energy for irreversible processes has form

$$\left(h_c + x^l \frac{\partial \beta_l}{\partial t} \right) = 0$$

Without additional conditions is valid for isentropic flow only.



Application- isentropic flow

Example 1.

Isentropic flow $\dot{s} = 0$, $\frac{p}{\rho_0} = \left(\frac{\rho}{\rho_0}\right)^\kappa$, $c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s = \kappa \frac{p}{\rho} = \kappa \frac{p_0}{\rho_0} \Lambda$

$$\Lambda = 1 - \frac{\kappa - 1}{\kappa + 1} (\lambda_i)^2,$$

for $\lambda = \frac{v_i}{c^*}$... nondimensional velocity

$$c^{*2} = \frac{2\kappa}{\kappa + 1} \frac{p_0}{\rho_0} = \text{const} \quad \dots \text{critical speed of sound}$$

$$\rho = \rho_0 \Lambda^{\frac{1}{\kappa-1}} \quad \dots \text{density}$$

Application- isentropic flow

For stationary case $t = \text{const}$ has Bateman principle form
 [F. Maršík, J. Non-Equilib. Thermodyn., Vol. 14, 1989, No4]

$$\delta S = \delta \int_V p(\rho, s) dv = \int_V \left(\frac{\partial p}{\partial \rho} \right)_s \delta \rho dv = - \frac{c^{\star 2}}{\kappa} \int_V \rho \lambda_i \delta \lambda_i dv + B.C.$$

We consider potential flow $\lambda_i = \frac{\partial \varphi}{\partial x^i}$

$$\delta S = \int_V \frac{\partial}{\partial x^i} (\rho \lambda_i) \delta \varphi dv + \int_{\partial V} (q_i - \rho \lambda_i) \delta \varphi da_i = 0$$

... balance of mass for stationary potential flow

$$\frac{\partial}{\partial x^i} (\rho \lambda_i) = 0, x \in V, \quad \varphi = \varphi_0, x \in \partial V_1, \quad \frac{\partial \varphi}{\partial x^i} = q_i, x \in \partial V_2,$$

$$\partial V = \partial V_1 \cup \partial V_2$$

Limit to classical mechanics of single body

Example 2.

Classical mechanics of mass body

$$m = \int_V \rho_0 dv$$

Isentropic $\dot{s} = 0$, $T = \text{const}$, $\dot{\beta} = 0$... no friction

$$S = \int_{t_0}^{t_1} \int_V \rho l dv dt = \int_{t_0}^{t_1} \left[\frac{mv_i v^i}{2} - \phi(x) \right] dt = \int_{t_0}^{t_1} L(x, \dot{x}, t) dt$$

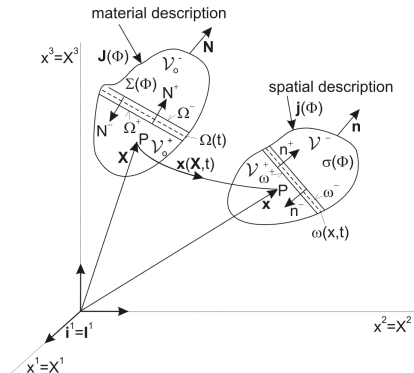
$$\delta S = \int_{t_0}^{t_1} \left(mv_i \frac{d}{dt} \delta x^i - \frac{\partial \phi}{\partial x^i} \delta x^i \right) dt =$$

$$= (mv_i \delta x^i) \Big|_{t_0}^{t_1} - \int_{t_0}^{t_1} \left[\frac{d}{dt} (mv_i) + \frac{\partial \phi}{\partial x^i} \right] \delta x^i dt = 0, \text{ for } v^i = \dot{x}^i = \frac{dx(t)}{dt}$$

Outline

- 1 Thermodynamic system - fundamental quantities
 - Thermodynamic states
- 2 Classical mechanics of mechanical systems
 - Conservation Laws
 - Canonical form of conservation laws-Poisson brackets
 - Thermodynamic systems beyond equilibrium
- 3 Variational formulation of Continuum Mechanics
 - Necessary condition for extremum
 - Balance of energy for irreversible processes
- 4 **Basic assumption of continuum thermodynamics**
 - Closing of the phenomenological theory
 - Thermodynamic Inequality-Constitutive equations
 - Maximum probability of state-Thermodynamic stability
- 5 Application to fluid flow stability

Balance laws-phenomenological approach



Balance of the quantity $\Phi(t)$ in the body with volume $\mathcal{V}_o = \mathcal{V}_o^+ + \mathcal{V}_o^-$
 ($\mathcal{V} = \mathcal{V}^+ + \mathcal{V}^-$) in which is some moving area of discontinuity $\Omega(X, t)$
 resp. $\omega(x, t)$

BALANCE LAWS

$$\frac{d\Phi(t)}{dt} = \dot{\Phi} = \mathcal{J}(\Phi) + \mathcal{P}(\Phi)$$

$$\mathcal{J}(\Phi) = \int_{\partial\mathcal{V}_o} J^K(\Phi) dA_K = \int_{\partial\mathcal{V}} j^k(\Phi) da_k,$$

$$\mathcal{P}(\Phi) = \int_{\mathcal{V}_o - \Omega} \Sigma(\Phi) d\mathcal{V} = \int_{\mathcal{V} - \omega} \sigma(\Phi) dv,$$

Balance laws and additional axioms

COMPLEX DESCRIPTION OF A REAL PHYSICAL SYSTEM V BALANCE LAWS + ADDITIONAL ASSUMPTIONS (AXIOMS)

Balance laws - definition of corresponding quantities

$$\phi = \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ \mathbf{x} \times \rho \mathbf{v} \\ \frac{\rho v^2}{2} \\ \rho U \\ \rho S \end{pmatrix} \begin{array}{l} \text{- mass} \\ \text{- momentum} \\ \text{- momentum of momentum} \\ \text{- mechanical energy} \\ \text{- internal energy} \\ \text{- entropy} \end{array}$$

$$\text{Global form } \dot{\Phi} + J(\phi) = P(\phi)$$

$$\text{Local form } \dot{\phi} + \nabla j(\phi) = \sigma(\phi)$$

Balance of mass and momentum

Balance of Mass $\dot{\rho} + \rho \frac{\partial v_l}{\partial x^l} = 0,$

Balance of Momentum $\rho \dot{v}^i + \frac{\partial t^{il}}{\partial x^l} = \rho f^i$

Balance of Moment of Momentum $t^{ij} = t^{ji}$

Balance of Mechanical Energy

$$\rho \left(\frac{\dot{v}^2}{2} \right) - \frac{\partial (t^{il} v_l)}{\partial x^i} + t^{il} \frac{\partial v_l}{\partial x^i} = \rho f^i v_i$$

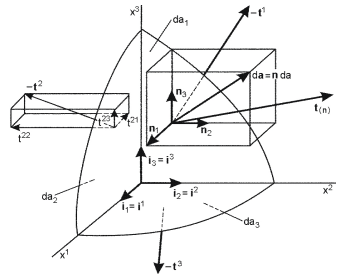
Balance of Internal Energy

$$\rho \dot{u} + \frac{\partial q^l}{\partial x^l} - t^{il} \frac{\partial v_l}{\partial x^i} = \tilde{q}$$

$q...$ heat flux vector

$f...$ vector of external volume forces

$\tilde{q}...$ absorbed heat (e.g., radiation)



Balance of the surface forces on the surface of the elemental tetrahedron and demonstration of the strain tensor's components t^{ij}

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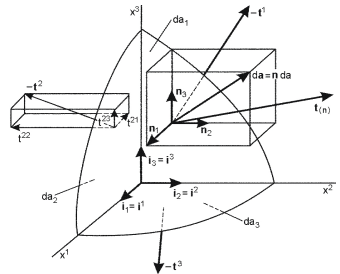
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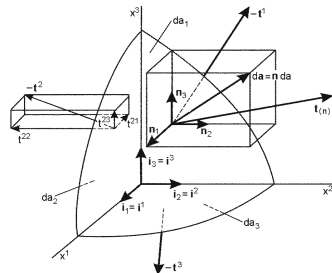
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Balance of the surface forces on the surface of the elemental tetrahedron and demonstration of the strain tensor's components t^{ij}

Axioms of- Time irreversibility and Maximum of probability of state

- **time irreversibility** - the processes taking place in the system which is not in any interaction with the surroundings do not allow the system to reach the initial state - II. Law of Thermodynamics which is formulated by means of the balance of entropy (*see later on*)

$$\pi = T\sigma(\mathcal{S}) = \rho(T\dot{s} - \dot{u}) - \frac{q^k}{T} \frac{\partial T}{\partial x^k} + t^{kl} \frac{\partial v_i}{\partial x^k} \geq 0$$

- density of energy dissipation (or production) is always positive

- **maximum of probability** - each material system exists in the state which is the most probable from all the possible states - entropy is a convex function of its variables and tends to its maximum

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BALANCE OF ENTROPY

General Balance Law

$$\frac{dS(t)}{dt} = \dot{S} = \mathcal{J}(S) + \mathcal{P}(S)$$

II. Law of Thermodynamics

$$\dot{S} - \mathcal{J}(S) = \mathcal{P}(S) \geq 0$$

Entropy flux definition

$$\mathcal{J}(S) = - \int_{\partial \mathcal{V}_o} \frac{Q^K}{T} dA_K + \int_{\mathcal{V}_o} \frac{\tilde{Q}}{T} d\mathcal{V} = - \int_{\partial \mathcal{V}} \frac{q^k}{T} da_k + \int_{\mathcal{V}} \frac{\tilde{q}}{T} dv,$$

Entropy production—consequence

$$\mathcal{P}(S) = \int_{\mathcal{V}_o - \Omega} \Sigma(S) d\mathcal{V} = \int_{\mathcal{V} - \omega} \sigma(S) dv \geq 0,$$

Fundamental Thermodynamic Inequality-Definition of Entropy

$$\pi = T\sigma(S) = \rho(T\dot{s} - \dot{u}) - \frac{q^k}{T} \frac{\partial T}{\partial x^k} + t^{kl} \frac{\partial v_i}{\partial x^k} \geq 0$$

Free Energy-thermodynamic potential depending on well defined quantities

$T, \rho, \frac{\partial T}{\partial x^i}, d_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial v_j} + \frac{\partial v_j}{\partial v_i} \right)$, stress tensor is split into elastic and dissipative part $t^{kl} = t_{el}^{kl} + t_{dis}^{kl}$ $f = f(T, \rho, \frac{\partial T}{\partial x^i}, d_{ij}) = u - Ts$ and $\dot{u} = \dot{f} + T\dot{s} + s\dot{T}$, Fundamental inequality gives

$$\pi = -\rho \left(\frac{\partial f}{\partial T} + s \right) \dot{T} + \left(t_{el}^{kl} + \rho^2 \frac{\partial f}{\partial \rho} \delta^{kl} \right) d_{ij} + t_{dis}^{ij} d_{ij} - \frac{q^i}{T} \frac{\partial T}{\partial x^i} - \rho \frac{\partial f}{\partial \left(\frac{\partial T}{\partial x^i} \right)} \frac{\partial T}{\partial x^i} - \rho \frac{\partial f}{\partial d_{ij}} \dot{d}_{ij} \geq 0.$$

Fundamental Thermodynamic Inequality has to be valid for all changes of

$$\dot{T}, d_{ij}, \frac{\partial T}{\partial x^i}, \dot{d}_{ij}.$$

To satisfy the **Fundamental Thermodynamic Inequality**-the following identity has to be fulfilled

$$s = - \left(\frac{\partial f}{\partial T} \right), \quad t_{cl}^{kl} = -p\delta_{kl} = -\rho^2 \left(\frac{\partial f}{\partial \rho} \right) \delta_{kl} = \left(\frac{\partial f}{\partial (1/\rho)} \right) \delta_{kl}, \quad \frac{\partial f}{\partial \left(\frac{\partial T}{\partial x^i} \right)} = 0, \quad \frac{\partial f}{\partial d_{ij}} = 0.$$

Free energy and entropy are defined as follows

$$\dot{f} = \dot{f}(T, \rho) = -s\dot{T} - p \left(\frac{\dot{1}}{\rho} \right) = \dot{u} - T\dot{s} - s\dot{T}, \quad \dot{s} = \frac{\dot{u}}{T} + \frac{p}{T} \left(\frac{\dot{1}}{\rho} \right)$$

Constitutive relations for thermo-viscous fluids can depend on the independent quantities [Coleman, Noll: Arch. Rat. Mech Analysis, vol.6, 1960] $T, \rho, \frac{\partial T}{\partial x^i}, d_{ij}$, as follows

$f = f(T, \rho), s = s(T, \rho), q^i = q^i(T, \rho, \frac{\partial T}{\partial x^i}, d_{ij}), t^{ij} = t^{ij}(T, \rho, \frac{\partial T}{\partial x^i}, d_{ij})$
 together with the **dissipation condition**

$$\pi = -\frac{q^k}{T} \frac{\partial T}{\partial x^k} + t_{dis}^{kl} d_{kl} \geq 0$$

The general form of the **dissipation condition** comprise all transport processes in fluids (including chemical reactions and phase transitions).

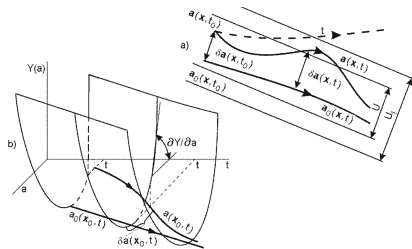
Thermodynamical flux J_i	Thermodynamical force X_i	Physical process
q^k	$\frac{\partial}{\partial x^k} \left(\frac{1}{T} \right)$	heat conductance
$\frac{t_{dis(l)}}{3}$	$\frac{1}{T} d_{(l)}$	volume viscosity
$\begin{matrix} (o)ij \\ t_{dis} \end{matrix}$	$\frac{1}{T} d_{ij}^{(o)}$	shear viscosity
$J_{D\alpha}^i$	$\frac{\partial}{\partial x^i} \left(\frac{\mu_\alpha}{T} \right) - \frac{F_\alpha^i}{T}$	diffusion
w_ρ	$A_\rho = -\sum_\alpha \nu_{\rho\alpha} M_\alpha \mu_\alpha$	chemical reaction, phase transition

Thermodynamical fluxes J_α and thermodynamical forces X_α following from the density of entropy production, for $l, j, k = 1, 2, 3$.

Quantities $d_{(l)}^{(o)ij}, t_{dis(l)}^{(o)}, t_{dis}^{(o)}, d_{ij}^{(o)}, J_{D\alpha}^i, w_\rho, A_\rho$ are defined by the balance laws of mass, momentum, energy and entropy: $\dot{S} - J(S) = P(S) = \sum_j J_j X_j \geq 0, \quad J_i = \sum_j L_{ij} X_j$



Ljapunov function of stability



Demonstration of Ljapunov's stability of the reference state $\mathbf{a}_o(\mathbf{x}, t)$ with respect to the fluctuations $\delta\mathbf{a}(\mathbf{x}, t)$

a) Stable state with regard to the fluctuation $\delta\mathbf{a}(\mathbf{x}, t_0)$ at the time t_0 (solid line), unstable state (dashed line)

b) Ljapunov's function $Y(\mathbf{x})$ for the states $\mathbf{a}_o(\mathbf{x}, t)$ at some fixed point \mathbf{x}_o

Function of these properties is e.g. internal energy $u = u(T, \rho)$

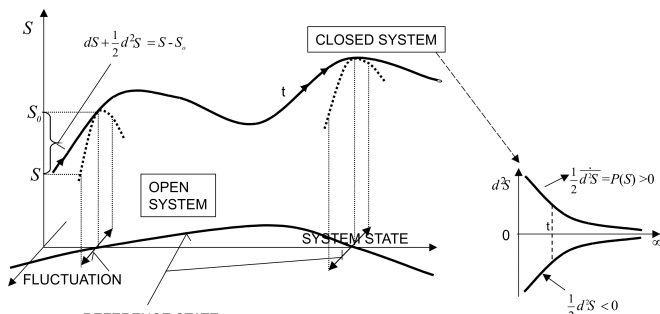
ENTROPY - CONVEX FUNCTION

Entropy is a convex function of the following variables:

u ... internal energy

v, \mathbf{e}_{ij} ... specific volume, deformation

n_α ... molar concentration



THERMODYNAMIC STABILITY CONDITIONS 1.

Internal energy is a function of two independent variables s , $1/\rho$, see the entropy definition for fluids

$$\dot{u} = \left(\frac{\partial u}{\partial s} \right) \dot{s} + \left(\frac{\partial u}{\partial \left(\frac{1}{\rho} \right)} \right) \left(\frac{\dot{1}}{\rho} \right) = T \dot{s} - p \left(\frac{\dot{1}}{\rho} \right).$$

In reference state denoted by "0" has the **Thermodynamic inequality** form

$$-\dot{u}_0 + T_0 \dot{s}_0 - p_0 \left(\frac{\dot{1}}{\rho_0} \right) + \frac{\pi}{\rho_0} = \frac{\pi}{\rho_0} \geq 0.$$

Provided that the independent quantity s , $1/\rho$ fluctuate around the reference state $s = s_0 + \delta s$, $\rho = \rho_0 + \delta \rho$ the internal energy deviates from reference state, see Fig.

$$u(T, \rho) = u_0 + du|_0 + \frac{1}{2} d^2 u|_0 + \dots$$



THERMODYNAMIC STABILITY CONDITIONS 2.

The **Thermodynamic inequality** with fluctuations δs , $\delta \rho$ around the reference state can be written as

$-\dot{u} + T_0 \dot{s} - p_0 \left(\frac{1}{\rho} \right) = \frac{\pi}{\rho_0} \geq 0$. The energy of dissipation $\frac{\pi}{\rho_0}$ at the left hand side of inequality is included in the energy of fluctuations, so that

$$-\dot{u}_0 - \overline{d\dot{u}|_0} - \frac{1}{2} \overline{d^2 \dot{u}|_0} + T_0 \dot{s}_0 + T_0 \overline{d\dot{s}|_0} - p_0 \left(\frac{1}{\rho} \right) - p_0 \overline{d \left(\frac{1}{\rho} \right) |_0} = \frac{\pi}{\rho_0} \geq 0$$

With respect to the definition of entropy in **reference state**

$$-\dot{u}_0 + T_0 \dot{s}_0 - p_0 \left(\frac{1}{\rho} \right) = 0 \text{ and the differential in this state}$$

$$-\overline{d\dot{u}|_0} + T_0 \overline{d\dot{s}|_0} - p_0 \overline{d \left(\frac{1}{\rho} \right) |_0} = 0, \quad \text{the time derivative of the second differential of } u \text{ is}$$

$$-\frac{1}{2} \overline{d^2 \dot{u}|_0} = \frac{\pi}{\rho_0} \geq 0.$$



THERMODYNAMIC STABILITY CONDITIONS 3.

The Ljapunov function of stability has to satisfy two following conditions:

- i) $\frac{d^2 u|_0}{dt^2} \geq 0$, (for $\delta T = \delta \rho = 0$ is $d^2 u|_0 = 0$),
- ii) $\frac{d^2 u|_0}{dt^2} \leq 0$.

The Second differential of internal energy is the **Ljapunov function of stability** of state with respect to the small fluctuations around the reference state "0" for thermo/visco/elastic fluids and solids, [Glansdorf, Prigogine: Thermodynamic Stability of Structure..., Wiley, 1971].

For fluids with the constitutive relation (equation of state) $p = p(T, \rho)$ we obtain

$$d^2 u|_0 = \left(\frac{\partial T}{\partial s} \right)_{\rho_0} (\delta s)^2 + \left[\left(\frac{\partial T}{\partial(1/\rho)} \right)_{s_0} - \left(\frac{\partial p}{\partial s} \right)_{\rho_0} \right] \delta s \delta \rho - \left(\frac{\partial T}{\partial(1/\rho)} \right)_{s_0} \delta(1/\rho)^2 \geq 0.$$

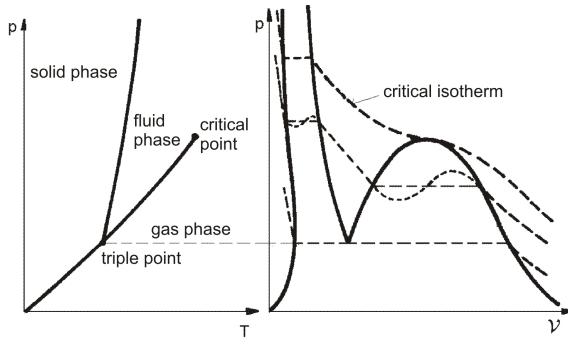
In the variables T , ρ has the Ljapunov function more simple form

$$d^2 u|_0 = \frac{C_v}{T} (\delta T)^2 - \chi (\delta(1/\rho))^2 > 0,$$

for isothermal compressibility $\chi = -\rho \left(\frac{\partial(1/\rho)}{\partial T} \right)_T$.



STABILITY OF THERMOVISCOUS FLUID



$p - T$ and $p - v$ diagrams of some material
solid lines - boundary curves, dashed lines - isotherms

BALANCE OF MASS AND MOMENTUM-ALTERNATIVE FORM

Balance of Mass $\dot{\rho} + \rho \frac{\partial v_l}{\partial x^l} = 0,$

Balance of Momentum $\rho \dot{v}^i + \frac{\partial t^{il}}{\partial x^l} = \rho f^i,$

Balance of Moment of Momentum $t^{ij} = t^{ji},$

Balance of Mechanical Energy $\rho \left(\frac{\dot{v}^2}{2} \right) - \frac{\partial (t^{il} v_l)}{\partial x^l} + t^{il} \frac{\partial v_i}{\partial x^l} = \rho f^i v_i,$

Balance of Total Enthalpy $\rho \dot{h}_{c0} - \frac{\partial p}{\partial t} + \frac{\partial q^l}{\partial x^l} - t^{il} \frac{\partial v_i}{\partial x^l} - v_i \frac{\partial t^{il}}{\partial x^l} = \tilde{q},$

where $h_{c0} = u + \frac{p}{\rho} + \frac{v^2}{2} + \phi,$ **q**... heat flux vector

f = $-\nabla \phi$... vector of external volume forces

\tilde{q} ... absorbed heat (e.g., radiation)

LOCAL FORM OF THE BALANCE OF ENTROPY

The fundamental thermodynamic inequality

$$\pi = T\sigma(S) = \rho(T\dot{s} - \dot{u}) - \frac{q^k}{T} \frac{\partial T}{\partial x^k} + t^{ki} \frac{\partial v_i}{\partial x^k} \geq 0$$

can be written as follows

$$\pi = \rho(T\dot{s} + \frac{1}{\rho} \frac{\partial p}{\partial t} - \dot{h}_c) + \bar{\pi} \geq 0$$

Modified energy of dissipation

$$\bar{\pi} = -\frac{q^k}{T} \frac{\partial T}{\partial x^k} + \frac{\partial(t_{dis}^{ki} v_i)}{\partial x^k} = \underbrace{-\frac{q^k}{T} \frac{\partial T}{\partial x^k}}_{>0} + \underbrace{v_i \frac{\partial t_{dis}^{ki}}{\partial x^k}}_{<>0} + \underbrace{t_{dis}^{ki} \frac{\partial v_i}{\partial x^k}}_{>0} \geq 0$$

for $\bar{\pi} < 0$... violation of thermodynamic inequality (possible onset of instability)

ENTROPY DEFINITION

follows from the law of the entropy balance equation

$$\pi = \rho_o \left[\underbrace{T_o(\dot{s}_o + \dot{\delta s}) + \frac{1}{\rho_o} \frac{\partial(p_o + \delta p)}{\partial t}}_0 - \dot{h}_{co} - \frac{d\dot{h}_{co}}{dt} - \frac{d^2 h_{co}}{2} \right] \geq 0$$

i.e.:

$$\dot{h}_{co} = T\dot{s} + \frac{1}{\rho_o} \frac{\partial p_o}{\partial t} \dots$$

} reference state (entropy definition)

$$\delta \dot{h}_{co} = T\delta \dot{s} + \frac{1}{\rho_o} \frac{\partial \delta p}{\partial t} \dots$$

- for isentropic $\dot{s} = 0$ and steady case $\dot{h}_c = 0$.

Total enthalpy is constant for a given material point.



STABILITY CONDITION OF THERMODYNAMIC PROCESSES

Le Châtelier - Braun principle

A spontaneous process induced by a deviation from a stable reference state (in the original work (1988) - equilibrium state) must be in a direction to restore the system in the stable reference (equilibrium) state.

$$\rho \left[\underbrace{T_o \frac{\dot{(s_o + \delta s)}}{\rho_o} + \frac{1}{\rho_o} \frac{\partial (p_o + \delta p)}{\partial t} - \dot{h}_{co} - \dot{d}h_{co} - \frac{1}{2} \dot{d}^2 h_{co}}_{0 \dots \text{reference state}} \right] = - \frac{1}{2} \dot{d}^2 h_{co} = \bar{\pi} > 0$$

The energy of fluctuation is dissipated by relaxation (transport) processes.

II. LAW OF THERMODYNAMICS - FINAL FORM

The final form of the II. Law of Thermodynamics can be interpreted as the balance of fluctuation energy and dissipation

$$\underbrace{-\frac{\rho_0}{2} \overline{d^2 h_{co}}}_{\text{energy of fluctuations}} = \underbrace{\tilde{\pi}}_{\text{dissipation processes}} \geq 0$$

$$\overline{d^2 h_{co}} = \frac{c_p}{T} \overline{(\delta T)^2} - \frac{1}{\rho^2 c^2} \frac{\partial(\delta p)^2}{\partial t} = \frac{2\tilde{\pi}}{\rho} \leq 0, \quad \text{for } c^2 = \left(\frac{\partial p}{\partial \rho}\right)_s$$

Ljapunov function of stability for the problems with convection is

$$d^2 h_{co} = \frac{c_p}{T} (\delta T)^2 - \frac{1}{\rho^2 c^2} (\delta p)^2 = \frac{c_p}{T} \left[(\delta T)^2 - \frac{T}{c_p (\rho c)^2} (\delta p)^2 \right] \geq 0.$$

Unstable for all fluctuation of pressure; the liquids are more stable $\frac{T}{c_p (\rho c)^2} \ll 1$

CONSTITUTIVE RELATIONS FOR THERMO-VISCOELASTIC FLUIDS

Heat flux

$$q_i = -\lambda(\rho, T) \frac{\partial T}{\partial x^i}$$

Stress tensor

$$t_{ij} = \underbrace{-p(\rho, T)\delta_{ij}}_{t_{ijel}} + \underbrace{\mu(\rho, T) \left(\frac{\partial v^i}{\partial x^j} + \frac{\partial v^j}{\partial x^i} - \frac{2}{3} \frac{\partial v^l}{\partial x^l} \delta_{ij} \right)}_{t_{ijdis}}$$

elastic part

dissipation part

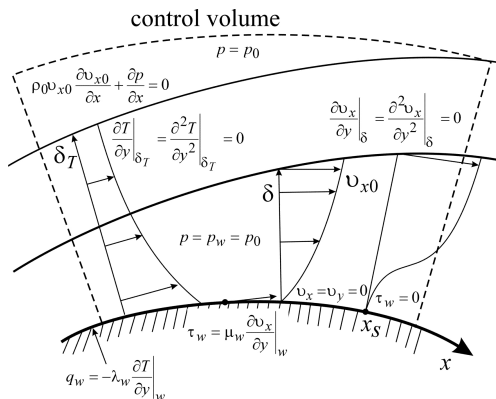
Total enthalpy

$$h_c(s, p) = u + \frac{p}{\rho} + \frac{v^2}{2} + \phi$$

potential energy
 kinetic energy
 pressure energy
 internal energy

CONSEQUENCES OF THE THERMODYNAMIC STABILITY CONDITIONS

Thermodynamic criterion of a boundary layer stability



Outline

- 1 Thermodynamic system - fundamental quantities
 - Thermodynamic states
- 2 Classical mechanics of mechanical systems
 - Conservation Laws
 - Canonical form of conservation laws-Poisson brackets
 - Thermodynamic systems beyond equilibrium
- 3 Variational formulation of Continuum Mechanics
 - Necessary condition for extremum
 - Balance of energy for irreversible processes
- 4 Basic assumption of continuum thermodynamics
 - Closing of the phenomenological theory
 - Thermodynamic Inequality-Constitutive equations
 - Maximum probability of state-Thermodynamic stability
- 5 **Application to fluid flow stability**

FLUID FLOW STABILITY

$$-\frac{\rho}{2} \dot{d^2 h_c} = \tilde{\pi}_{B.L} = -\frac{q_y}{T} \frac{\partial T}{\partial y} + t_{x,y,dis} \frac{\partial v_x}{\partial y} + v_x \frac{\partial}{\partial y} t_{x,y,dis} \geq 0$$

for

$$t_{x,y,dis} = \mu \frac{\partial v_x}{\partial y}, \quad q_y = -\lambda \frac{\partial T}{\partial y}$$

$$\tilde{\pi}_{B.L} = +\frac{\lambda}{T} \left(\frac{\partial T}{\partial y} \right)^2 + \mu \left(\frac{\partial v_x}{\partial y} \right)^2 + v_x \left(\frac{\partial \mu}{\partial y} \frac{\partial v_x}{\partial y} + \mu \frac{\partial^2 v_x}{\partial y^2} \right) \geq 0$$

To preserve the fluid flow stability (fluctuations of total enthalpy do not increase infinitely) a molecular viscosity $\mu = \mu(\rho, T)$ changes for intensive momentum transfer to turbulent viscosity $\mu \rightarrow \mu_{turb}(y)$ and depends implicitly on the flow field configuration.

FLUID FLOW STABILITY

Definition of entropy

$$T\dot{s} = \dot{h}_c - \frac{1}{\rho} \frac{\partial p}{\partial t} h = u + \frac{p}{\rho} + \frac{v^2}{2} + \varphi \quad \dots \text{specific total enthalpy}$$

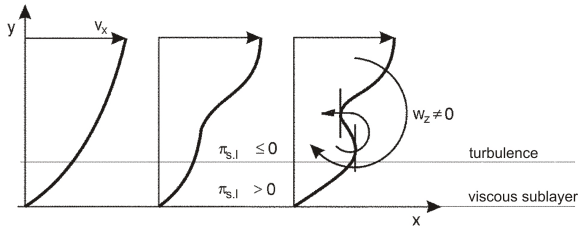
Thermodynamic condition of boundary layer stability $v_x = v_x(x, y)$

$$-\frac{\rho}{2} \frac{\dot{h}_c}{\rho} = \lambda \left(\frac{\partial T}{\partial y} \right)^2 + \mu \left(\frac{\partial v_x}{\partial y} \right)^2 + \mu v_x \left[\frac{d \ln \mu}{dT} \frac{\partial T}{\partial y} \frac{\partial v_x}{\partial y} + \frac{\partial^2 v_x}{\partial y^2} \right] \geq 0$$

Thermodynamic condition of stability is the extension of the **Rayleigh condition of stability**, which has the form

$$\frac{\partial^2 v_x}{\partial y^2} > 0 \quad \text{everywhere in a boundary layer}$$

STABILITY OF THERMOVISCOUS FLUID WITH CONVECTION

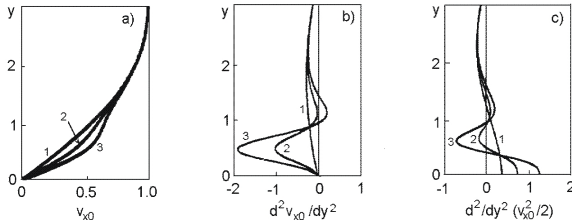


Disturbance of the velocity profile at the boundary layer causing the loss of stability ($\tilde{\pi}_{s,l} < 0$).

Perpendicular component of the vorticity

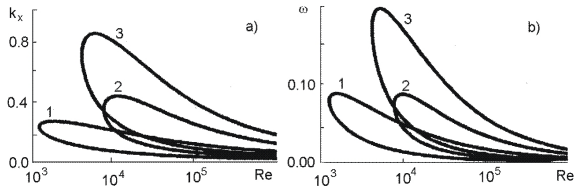
$$w_z = \text{rot } |\mathbf{v}|_z \approx -\partial v_x / \partial y$$

VELOCITY PROFILES AT BOUNDARY LAYER



- a) 1 - Polhausen's velocity profile for $a = 1 \dots$, i.e.
 $v_{x0}(x, y) = 2(y/\delta_{m.v}) - 2(y/\delta_{m.v})^3 + (y/\delta_{m.v})^4$, 2, 3 - the velocity profiles 1 with disturbances
- b) Course of the Rayleigh's criterion of stability
- c) Course of the thermodynamic criterion of stability of the process

LIMIT ON STABILITY OF SMALL DISTURBANCES FOR VELOCITY PROFILES



Limit on stability of small disturbances for the velocity profiles depending up $Re = v_{x\infty} \delta^* / \nu$

The areas within the curves are the areas of the instability

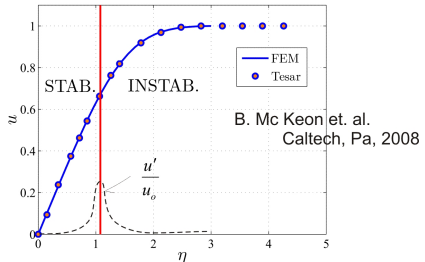
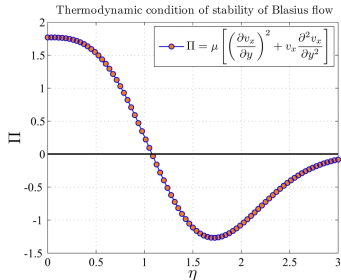
a) For the waves lengths $l_x = 2\pi\delta^* / k_x$

b) For the frequency $f = \omega v_{z\infty} / (2\pi\delta^*)$

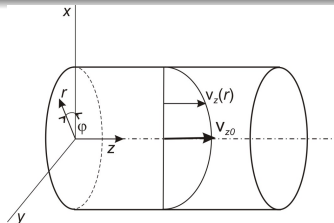
BLASIUS FLOW

Incompressible fluid flow past plate without pressure gradient.

$$u = \frac{v_{x0}}{v_{x\infty}} = f(\eta), \quad \eta = \sqrt{\frac{v_{x\infty}}{\nu}} \frac{y}{2\sqrt{x}}$$



VISCOUS POISSEUILLE FLOW



$$v_r = 0, \quad v_\varphi = 0, \quad v_z = v_z(r)$$

$$\frac{\partial p}{\partial z} = \frac{\nu}{r} \frac{d}{dr} \left(r \frac{dv_z}{dr} \right) = A_p = \text{const} \quad (\text{or } p = A_p z + B_p)$$

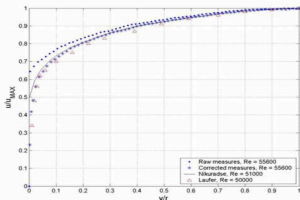
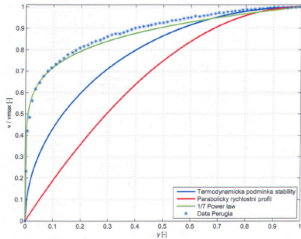
$$\frac{v_z}{v_{z0}} = f(r) = 1 - r^2, \quad r = \frac{r}{R_2}, \quad v_{z0} = -\frac{1}{4\rho\nu^2} \frac{\partial p}{\partial z}$$

by Rayleigh criterion $\frac{\partial^2 f}{\partial r^2} = -2$ is stable

by Thermodynam. criterion

$$\Pi = \frac{\pi R_2^2}{\mu v_{z0}^2} = \frac{1}{r} \frac{\partial}{\partial r} \left[r f(r) \frac{\partial f(r)}{\partial r} \right] = -4(1 - 2r^2) > 0 \quad \text{is partially stable}$$

POISSEUILLE FLOW STABILITY



Poiseuille flow is stable for $r > 1/\sqrt{2}$,

Globally is marginally stable i.e.: $2\pi \int_0^1 \Pi_p r dr = 2\pi \int_0^1 4(\dots)$

wall shear stress is $\tau_w = -\frac{\eta v_{z0}}{2R_2}$

turbulent flow $\frac{v_z(r)}{v_{z0}} = y^{1/7}$, $y = 1 - r$, $r = r/R_2$,

by Rayleigh criterion $\frac{\partial^2 f}{\partial r^2} = -\frac{6}{49(1-r)^{13/7}}$ is stable
 by Thermodynam. criterion

$$\Pi = \frac{1}{r} \frac{\partial}{\partial r} [r f(r) \frac{\partial f(r)}{\partial r}] = -\frac{2}{49r(1-r)^{5/7}} < 0$$

is completely unstable

thermo. unstable flow

$$\frac{v_z(r)}{v_{z0}} = \sqrt{1 - r^2}, \quad r = r/R_2,$$

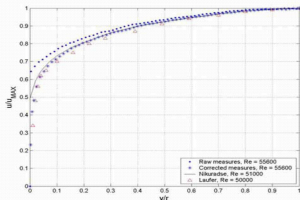
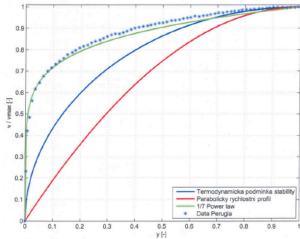
Globally is unstable $2\pi \int_0^1 \Pi_{\text{Term}} r dr = -2\pi < 0$,

wall shear stress is $\tau_w = -\frac{\eta v_{z0}}{R_2} \frac{r}{\sqrt{1-r^2}} \Big|_{r \rightarrow 1} \rightarrow \infty$

(P. Novotný, 2008, CTU Prague)



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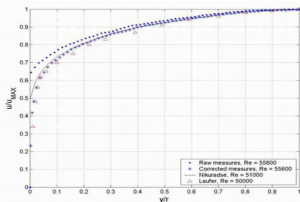
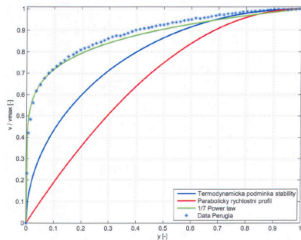
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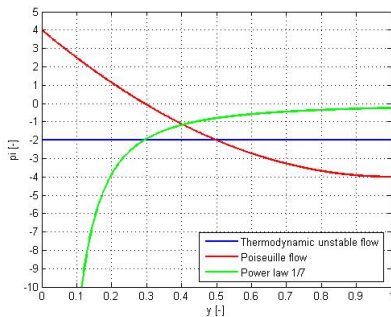
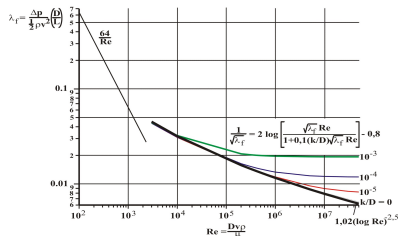
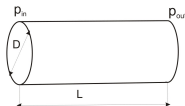
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(P. Novotný, 2008, CTU Prague)



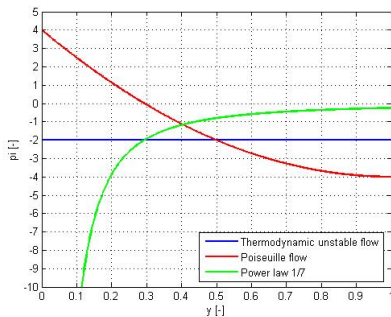
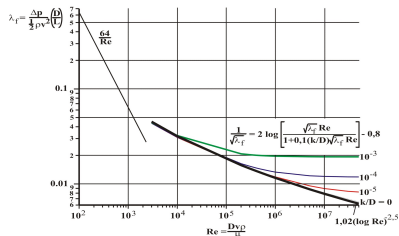
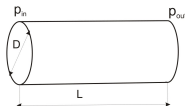
TUBE FLOW

TUBE FLOW



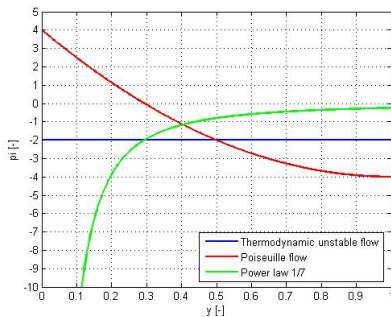
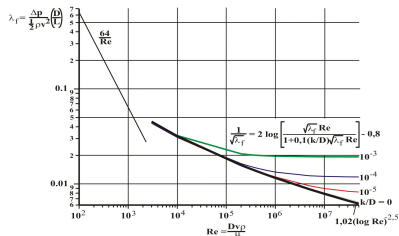
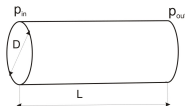
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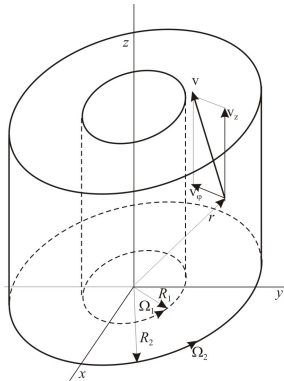


TUBE FLOW

TUBE FLOW



COUETTE FLOW



velocity field

$$\mathbf{v} = (0, v_\varphi(r), v_z(r))$$

$$\Omega(r) = A + \frac{B}{r^2}$$

$$A = -\Omega_1 \eta^2 \frac{1 - \mu / \eta^2}{1 - \eta^2}$$

$$B = \Omega_1 \frac{R_1^2 (1 - \mu)}{1 - \eta^2}$$

$$\mu = \Omega_2 / \Omega_1, \quad \eta = R_1 / R_2$$

VISCOUS COUETTE FLOW

$$v_r = v_z = 0, \quad v_\varphi = v_\varphi(r)$$

$$\frac{d}{dr} \left(\frac{p}{\rho} \right) = \frac{v_\varphi}{r}, \quad \nu \left(\nabla^2 v_\varphi - \frac{v_\varphi}{r^2} \right) = \nu \frac{d}{dr} \left(\frac{d}{dr} + \frac{1}{r} \right) v_\varphi = 0$$

$$v_\varphi = Ar + \frac{B}{r} = \omega(r) \cdot r, \quad \omega(r) = A + \frac{B}{r^2}$$

(S. Chandrasekhar, Hydrodyn. and Hydromag. Stability, Oxford, 1961)

STABILITY CRITERIA FOR COUETTE FLOW

$$-\infty < \mu = \Omega_2/\Omega_1 < 1, \quad 0 < \eta = R_1/R_2 < 1, \quad 0 < \tilde{r} = r/R_2 < 1$$

Rayleigh criterion gives

$$\Phi(r) = 4A \left(A + \frac{B}{r^2} \right) \stackrel{r=R_2\tilde{r}}{=} \bar{\Omega}_R (\mu - \eta^2) [\eta^2(1 - \mu) + \tilde{r}^2(\mu - \eta^2)] \geq 0$$

for $\bar{\Omega}_R = \frac{4\Omega_1^2}{\tilde{r}^2} (1 - \eta^2)^2 > 0$, for $0 < \mu < 1$, $\mu = \Omega_2/\Omega_1 > \eta^2$,
for $\mu < 0$ $\mu(\tilde{r}^2 - \eta^2) < \eta^2(\tilde{r}^2 - 1)$ no conclusion

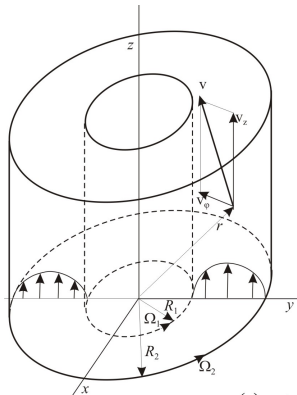
Thermodynamic criterion gives

$$\frac{\pi}{\mu} = \frac{2B}{r^2} \left(A + \frac{3B}{r^2} \right) \stackrel{r=R_2\tilde{r}}{=} \bar{\Omega}_T (1 - \mu) [3\eta^2 + \tilde{r}^2(\mu - \eta^2)] \geq 0$$

for $\bar{\Omega}_T = \frac{2\Omega_1^2\eta^2}{\tilde{r}^4(1 - \eta^2)^2} > 0$, $-2\eta^2 < \mu \leq 1$, $\mu = \Omega_2/\Omega_1 > \eta^2$,

for $\mu < 0$, $\mu > \eta^2 - 3$

POISEUILLE AND COUETTE FLOW



velocity field

$$\mathbf{v} = (0, v_\varphi(r), v_z(r))$$

$$v_\varphi(r) = \omega(r) \cdot r$$

$$\omega(r) = A + \frac{B}{r^2}$$

$$A = -\Omega_1 \eta^2 \frac{1 - \mu / \eta^2}{1 - \eta^2}$$

$$B = \Omega_1 \frac{R_1^2 (1 - \mu)}{1 - \eta^2}$$

$$\mu = \Omega_2 / \Omega_1, \quad \eta = R_1 / R_2$$

$$v_z(r) = A_p R_2^2 \left\{ 1 - \left(\frac{r}{R_2} \right)^2 + \left[1 - \left(\frac{R_1}{R_2} \right)^2 \right] \frac{\ln \left(\frac{r}{R_2} \right)}{\ln \left(\frac{R_2}{R_1} \right)} \right\}, \quad \text{pro } A_p = -\frac{1}{4\mu} \left(\frac{\partial p}{\partial z} \right) \left[\frac{1}{\text{ms}} \right] = \text{const}$$



VISCOUS COUETTE FLOW AND POISEUILLE FLOW

Isothermal, incompressible fluid

Balance of mass

$$\frac{\partial v_r}{\partial r} + \frac{v_r}{r} + \frac{1}{r} \frac{\partial v_\theta}{\partial \theta} + \frac{\partial v_z}{\partial z} = 0$$

Balance of momentum

$$\begin{aligned} \frac{\partial v_r}{\partial t} + (\mathbf{v} \cdot \nabla) v_r - \frac{v_\theta^2}{r} &= -\frac{\partial}{\partial r} \left(\frac{p}{\rho} \right) + \nu \left(\nabla^2 v_r - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} - \frac{v_r}{r^2} \right) \\ \frac{\partial v_\theta}{\partial t} + (\mathbf{v} \cdot \nabla) v_\theta + \frac{v_r v_\theta}{r} &= -\frac{1}{r} \frac{\partial}{\partial \theta} \left(\frac{p}{\rho} \right) + \nu \left(\nabla^2 v_\theta + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} - \frac{v_\theta}{r^2} \right) \\ \frac{\partial v_z}{\partial t} + (\mathbf{v} \cdot \nabla) v_z &= -\frac{\partial}{\partial z} \left(\frac{p}{\rho} \right) + \nu \nabla^2 v_z \\ \mathbf{v} \cdot \nabla &= v_r \frac{\partial}{\partial r} + \frac{v_\theta}{r} \frac{\partial}{\partial \theta} + v_z \frac{\partial}{\partial z} \\ \nabla^2 &= \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2} \end{aligned}$$

STABILITY OF COUETTE AND POISSEUILLE FLOW

Thermodynamic stability criterion for Couette flow between two rotating coaxial cylinders

Rayleigh criterion $\Phi = \frac{1}{r^3} \frac{d}{dr} (r^2 \Omega)^2 > 0$ ($T = \text{const}$, $v_y = 0$)

Thermodynamic stability criterion for $T = \text{const}$

(F. Maršík, Continuum thermodynamics, Academia, Praha, 1999)

$$\begin{aligned} \frac{\pi}{\mu} = & v_\varphi \frac{d^2 v_\varphi}{dr^2} + \left(\frac{dv_\varphi}{dr} \right)^2 - \frac{2v_\varphi}{r} \frac{dv_\varphi}{dr} + \left(\frac{v_\varphi}{r} \right)^2 + \\ & + v_z \left(\frac{d^2 v_z}{dr^2} + \frac{1}{r} \frac{dv_z}{dr} \right) + \left(\frac{dv_z}{dr} \right)^2 \geq 0 \end{aligned}$$

STABILITY OF COUETTE AND POISSEUILLE FLOW

Thermodynamic stability condition - nondimensional form

$$\begin{aligned} & \text{for } r = r/R_2, \quad \eta = R_1/R_2, \quad \bar{\mu} = \Omega_2/\Omega_1, \\ & \frac{\pi}{\mu\Omega_1^2} [1] = \frac{2\eta^2(1-\bar{\mu})}{r^2(1-\eta^2)} \left[\frac{3\eta^2(1-\bar{\mu})}{r^2(1-\eta^2)} - \eta^2 \frac{1-\bar{\mu}/\eta^2}{1-\eta^2} \right] + \\ & + \text{CP} \left[8r^2 - 4 - 4 \frac{1+\eta^2}{\ln(\eta)} \ln r + \frac{4(1-\eta^2)}{\ln(\eta)} - \frac{(1-\eta^2)^2}{2r^2 \ln(\eta)} \right] \geq 0, \end{aligned}$$

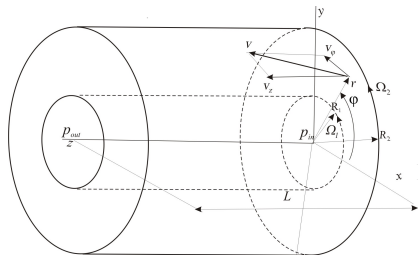
Coupling coefficient

$$\text{CP} = \left[\frac{(\mu - \eta^2)}{2\Omega_1 R_2^2} \right] \frac{\text{Re}}{S}.$$

(P. Novotný, 2008, CTU Prague)

(3)

VORTEX TUBE



Swirl number

$$S = \frac{2\pi \int_{R_1}^{R_2} \rho v_\phi v_z r dr}{2\pi R_2 \int_{R_1}^{R_2} \rho v_z^2 r dr}$$

Reynolds number

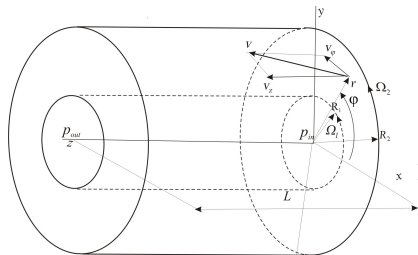
$$Re = \frac{2\bar{v}_z R_2}{\nu}, \text{ for } \bar{v}_z = \frac{2\pi \int_{R_1}^{R_2} v_z r dr}{\pi(R_2^2 - R_1^2)}$$

Coupling coefficient

$$CP = \left[\frac{(\mu - \eta^2)}{2\Omega_1 R_2^2} \right] \frac{Re}{S} \frac{S_1(\mu, \eta)}{\mathcal{R}(\eta) S_2(\eta)}$$

$$\frac{S_1(\mu, \eta)}{\mathcal{R}(\eta) S_2(\eta)} \Big|_{\eta=0.5, \bar{\mu}=0} = -0.337$$

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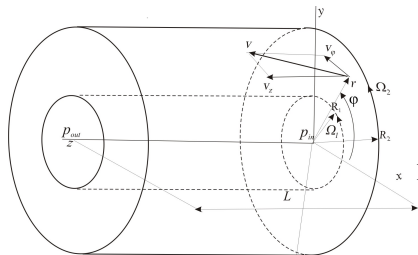
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Reynolds number

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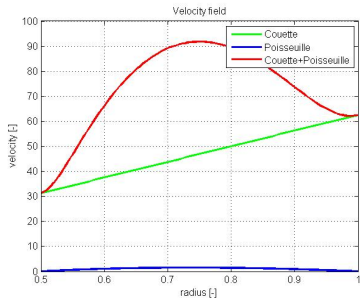
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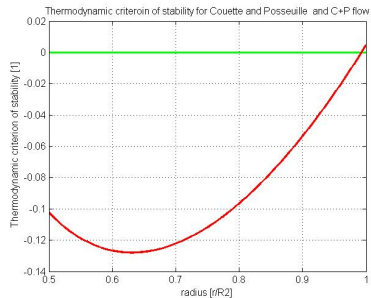
VORTEX TUBE

Stability of Poiseuille and Couette flow $Re = 40000$



Velocity profiles

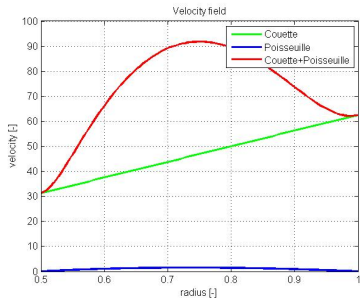
$$\Omega_1 = \Omega_2 = 2500[1/s]$$



Thermodynamic stability criterion for $\Omega_1 = \Omega_2 = 2500[1/s]$

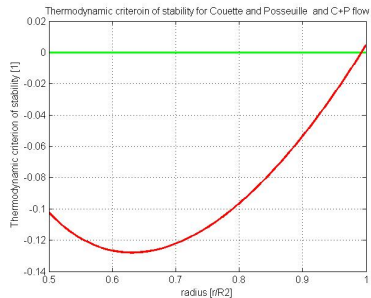
VORTEX TUBE

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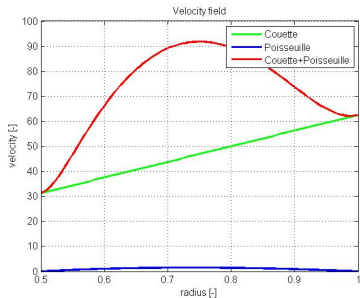


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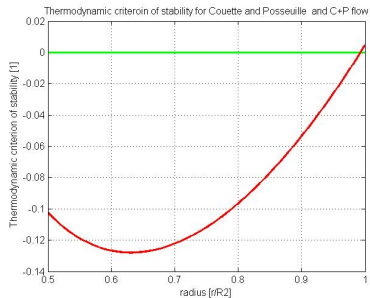
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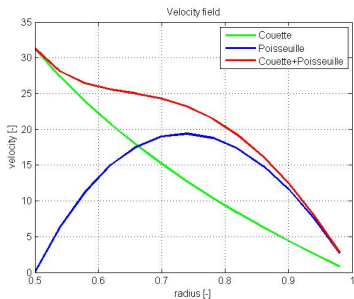


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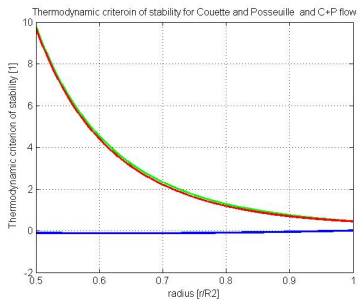
VORTEX TUBE

Stability of Poiseuille and Couette flow $Re = 40000$



Velocity profiles

$$\Omega_1 = 2500[1/s], \quad \Omega_2 = 0$$

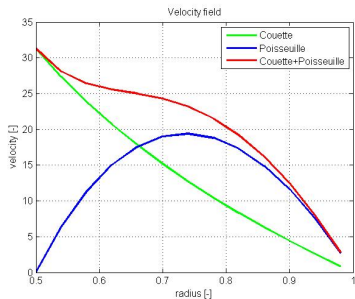


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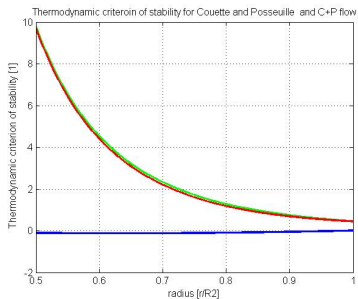
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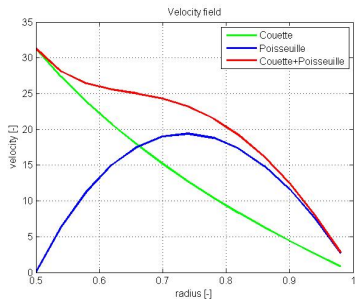


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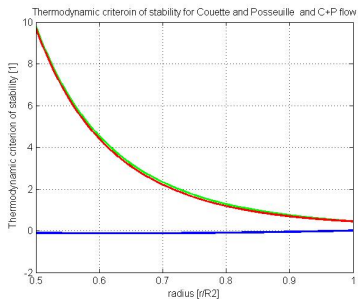
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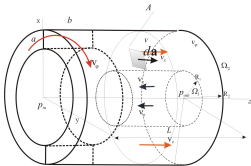
RANK-HILSCH VORTEX TUBE

Potential vortex $v_\theta = \frac{\Gamma_0}{r}$, $\Gamma_0 = \int_0^{2\pi} v_{\theta 2} r dr$

Balance of energy $h_c = c_p T + \frac{v_\theta^2}{2} = const$

$$T_1 - T_2 = -\frac{v_\theta^2}{2c_p} \left[\left(\frac{R_2}{R_1} \right)^2 - 1 \right] \doteq -60 \text{ K}$$

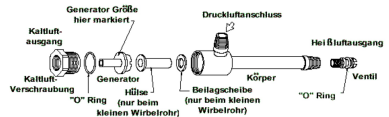
for tube $R_2/R_1 = 1.5$ and with air
 $c_p = 1000 \text{ [J/kg K]}$ $v_\theta = 310 \text{ [m/s]}$



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VORTEX TUBE

Temperature difference 46°C



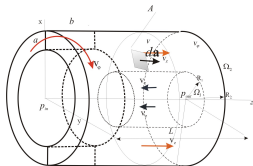
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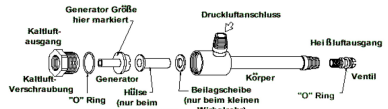
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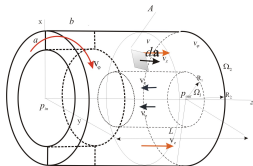
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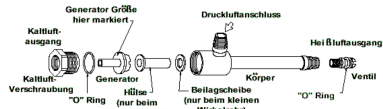
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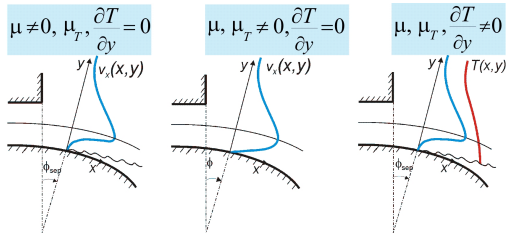


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HEATED WALL JET - THERMODYNAMIC CONDITION OF STABILITY



The thermodynamic condition of stability for a heated wall jet:

$$(\lambda + \lambda_T) \left(\frac{\partial T}{\partial y} \right)^2 + (\mu + \mu_T) \left(\frac{\partial v_x}{\partial y} \right)^2 + (\mu + \mu_T) v_x \left[\frac{d \ln(\mu + \mu_T)}{dT} \left(\frac{\partial T}{\partial y} \right) \left(\frac{\partial v_x}{\partial y} \right) + \frac{\partial^2 v_x}{\partial y^2} \right] \geq 0$$

> 0 > 0 for air is positive < 0 > 0 > 0 < 0

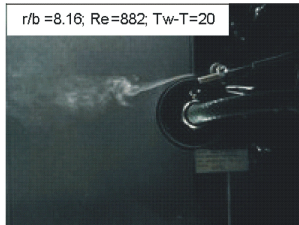
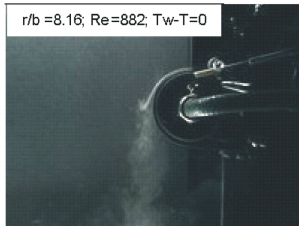
Possible conclusion:

Negative temperature gradient enhances the destabilization role of the term $(v_x - v_y) \frac{\partial^2 v_x}{\partial y^2}$, which is in competition of always positive term $(\lambda + \lambda_T) \left(\frac{\partial T}{\partial y} \right)^2$



Thermodynamic system - fundamental quantities
Classical mechanics of mechanical systems
Variational formulation of Continuum Mechanics
Basic assumption of continuum thermodynamics
Application to fluid flow stability
Conclusion

Application to tube flow stability
Application to Couette flow stability
Vortex tube
Stabilizing by temperature gradient



Outline

- 1 Thermodynamic system - fundamental quantities
 - Thermodynamic states
- 2 Classical mechanics of mechanical systems
 - Conservation Laws
 - Canonical form of conservation laws-Poisson brackets
 - Thermodynamic systems beyond equilibrium
- 3 Variational formulation of Continuum Mechanics
 - Necessary condition for extremum
 - Balance of energy for irreversible processes
- 4 Basic assumption of continuum thermodynamics
 - Closing of the phenomenological theory
 - Thermodynamic Inequality-Constitutive equations
 - Maximum probability of state-Thermodynamic stability
- 5 Application to fluid flow stability



Conclusion

- The stability of a state of a system is the fundamental condition of its existence, i.e.: $\ddot{S}|_o = \dot{J}(S)|_o + \dot{P}(S)|_o < 0$
- The origin of a new dissipative structure (e.g. in order to increase the stability) is accompanied by an increase of the entropy production $\dot{P}(S) > 0$ ($J(S) = \text{const}$, the so-called intensive growth). This growth has to be compensated by a closer interaction with its surroundings ($-\dot{J}(S) > 0$ the so-called extensive growth).
- The system goes to a thermodynamic equilibrium when it terminates its both intensive and extensive growth. All dissipative irreversible processes tend to zero.

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