Interaction of weak and strong discontinuities for two-component mixture separation

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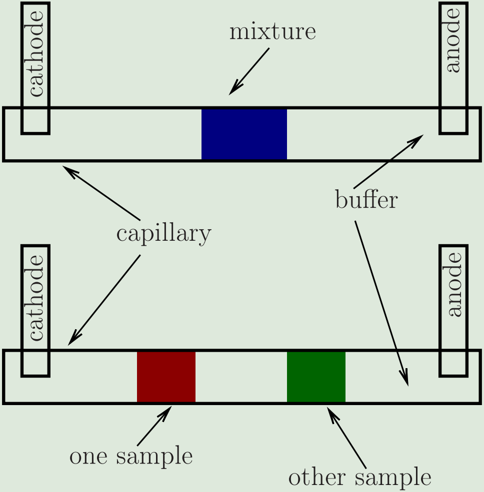
A schematic diagram of a capillary zone electrophoresis setup



The interior of capillary is filled with an electrolyte. The sample to be analyzed is injected in the capillary. Due to electric field it travels down the capillary and forms some zones. So we have some travelling zones and we can identify a mixture.

Mathematical model of capillary zone electrophoresis

System of two hyperbolic equations

$$\frac{\partial u^k}{\partial t} + \frac{\partial}{\partial x}\left(\frac{\mu^k u^k}{1+s}\right) = 0, \quad k = 1,2,$$

$$s = u^1 + u^2 > -1$$

Notations

u^k — «effective» concentrations,
μ^k — «effective» component mobilities,
s —conductivity of the mixture

System of two hyperbolic equations, written in the Riemann invariants

A change of variable $t \to \mu^1\mu^2 t$

$$\frac{\partial R^k}{\partial t} + \lambda^k(R^1,R^2)\frac{\partial R^k}{\partial x} = 0, \quad k = 1,2,$$

$$\lambda^1(R^1,R^2) = R^1R^1R^2, \quad \lambda^2(R^1,R^2) = R^2R^1R^2$$

Concentration expressed by Riemann invariants, $u = u(R)$

$$u^1 = \frac{\mu^2(R^1-\mu^1)(R^2-\mu^1)}{R^1R^2(\mu^1-\mu^2)}, \quad u^2 = \frac{\mu^1(R^1-\mu^2)(R^2-\mu^2)}{R^1R^2(\mu^2-\mu^1)}$$

$R = R(u)$ is the roots of characteristic polynomial

$$(1+u^1+u^2)(R)^2 - (\mu^1+\mu^2+u^1\mu^2+u^2\mu^1)R + \mu^1\mu^2 = 0$$

Riemann problem

Initial data

$$R^1\big|_{t=0} = R^1_0(x), \quad R^2\big|_{t=0} = R^2_0(x),$$

$$R^1_0(x) = \begin{cases} \mu^1, & x < x^1, \\ q^1, & x^1 < x < x^2, \\ \mu^1, & x^2 < x, \end{cases} \qquad R^2_0(x) = \begin{cases} \mu^2, & x < x^1, \\ q^2, & x^1 < x < x^2, \\ \mu^2, & x^2 < x, \end{cases}$$

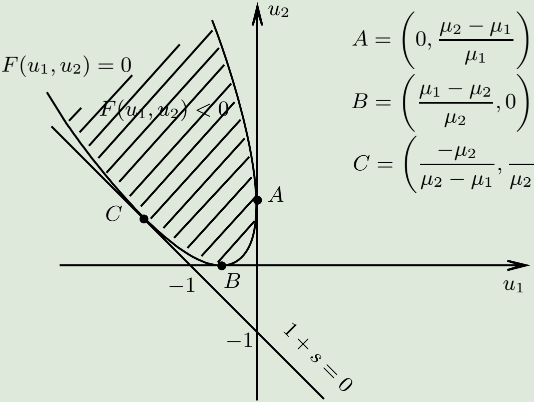
$$0 < q^1 < \mu^1 < \mu^2 < q^2$$

Rankine-Hugoniot conditions

$$D\left[\frac{(\mu^k - R^1)(\mu^k - R^2)}{\mu^k R^1 R^2}\right] = \left[(\mu^k - R^1)(\mu^k - R^2)\right], \quad k = 1,2$$

$$F(u_1,u_2) \equiv (\mu_1+\mu_2+u_1\mu_2+u_2\mu_1)^2 - 4(1+s)\mu_1\mu_2$$

- $F(u_1,u_2) > 0$, $1+s>0$ — hyperbolic type,
- $F(u_1,u_2) < 0$ — elliptic type



$$A = \left(0, \frac{\mu_2-\mu_1}{\mu_1}\right)$$

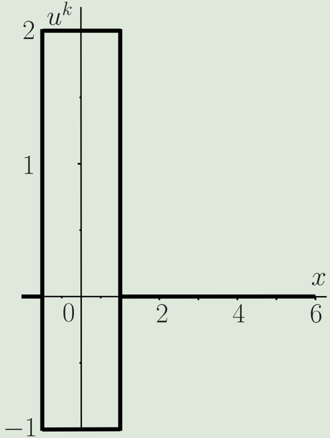
$$B = \left(\frac{\mu_1-\mu_2}{\mu_2}, 0\right)$$

$$C = \left(\frac{-\mu_2}{\mu_2-\mu_1}, \frac{\mu_1}{\mu_2-\mu_1}\right)$$

Parameters and initial conditions

$$u_0^1 = 2, \quad u_0^2 = -1, \quad x^1 = -1, \quad x^2 = 1$$

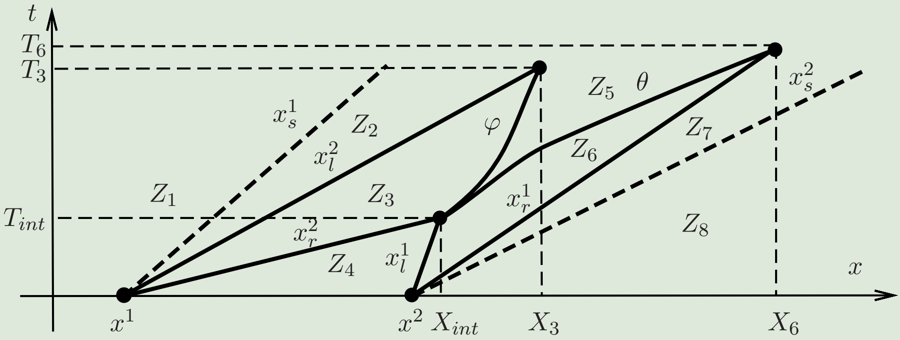
$$q^1 = 2, \quad \mu^1 = 5, \quad \mu^2 = 8, \quad q^2 = 10$$



Zone

$$\mathbb{Z}_k = \{R_k^1(x,t), R_k^2(x,t); a_k(t), b_k(t)\}$$

$a_k(t), b_k(t)$ — left and right border of zone,
$R_k^1(x,t), R_k^2(x,t)$ — Riemann invariants in zone



Evolution of initial discontinuities

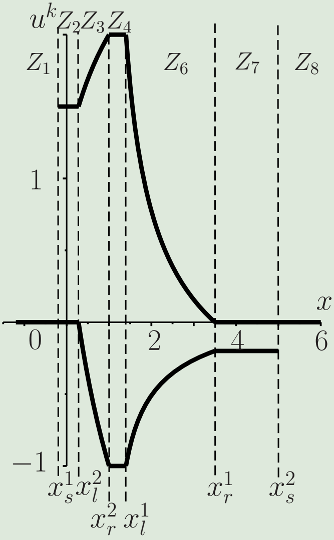
Solution at the moment $t = +0$

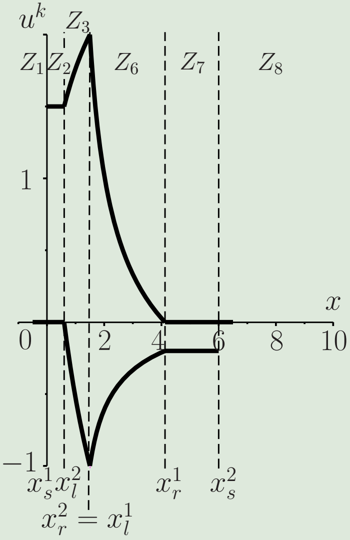
$$\mathbb{Z}_1 = \{\mu^1, \mu^2; -\infty, x_s^1(t)\}, \quad \mathbb{Z}_2 = \{q^1, \mu^2; x_s^1(t), x_l^2(t)\},$$
$$\mathbb{Z}_3 = \{q^1, R_a^2(z^2); x_l^2(t), x_r^2(t)\}, \quad \mathbb{Z}_4 = \{q^1, q^2; x_r^2(t), x_l^1(t)\},$$
$$\mathbb{Z}_6 = \{R_a^1(z^1), q^2; x_l^1(t), x_r^1(t)\}, \quad \mathbb{Z}_7 = \{\mu^1, q^2; x_r^1(t), x_s^2(t)\},$$
$$\mathbb{Z}_8 = \{\mu^1, \mu^2; x_s^2(t), +\infty\},$$
$$R_a^1(z^1) = \sqrt{\frac{z^1}{q^2}}, \quad z^1(x,t) = \frac{x - x^2}{t}, \quad R_a^2(z^2) = \sqrt{\frac{z^2}{q^1}}, \quad z^2(x,t) = \frac{x - x^1}{t}$$

Strong waves and rarefaction waves

$$x_s^1 = x^1 + q^1\mu^1\mu^2 t, \quad x_s^2 = x^2 + \mu^1\mu^2 q^2 t, \quad D^1 = q^1\mu^1\mu^2, \quad D^2 = \mu^1\mu^2 q^2;$$
$$x_l^1 = x^2 + q^1 q^1 q^2 t, \quad x_r^1 = x^2 + \mu^1\mu^1 q^2 t,$$
$$x_l^2 = x^1 + q^1\mu^2\mu^2 t, \quad x_r^2 = x^1 + q^1 q^2 q^2 t$$

Evolution of initial discontinuities at the moment $t = +0$





Interaction between two rarefaction waves

The point of interaction is the solution of equation $x_r^2(t) = x_l^1(t)$

$$T_{int} = \frac{x^2 - x^1}{q^1 q^2 (q^2 - q^1)}, \quad X_{int} = \frac{x^1 q^1 - x^2 q^2}{q^1 - q^2}$$

Zones

Zone $\mathbb{Z}_4$ disappears, new zone $\mathbb{Z}_5$ appears and border of zone $\mathbb{Z}_3$ and $\mathbb{Z}_6$ are changed

$$\mathbb{Z}_5 = \{R^1(x,t), R^2(x,t); \varphi(t), \theta(t)\}$$

$$\mathbb{Z}_3 = \{q^1, R_a^2(z^2)); x_l^2(t), \varphi(t)\}, \quad \mathbb{Z}_6 = \{R_a^1(z^2), q^2, \theta(t), x_r^1(t)\}$$

Functions $\varphi(t)$, $\theta(t)$

Line $\varphi(t)$ is the weak discontinuity of Riemann invariant R^1. For determing $\varphi(t)$ one have the Cauchy problem

$$\frac{d\varphi}{dt} = \lambda^1(q^1, R_a^2), \quad \varphi(T_{int}) = X_{int}$$

The solution is

$$\left(\varphi - x^1\right)^{1/2} = \left(q^1\right)^{3/2}\left(t^{1/2} - T_{int}^{1/2}\right) + \left(X_{int} - x^1\right)^{1/2}$$

For weak discontinuity $x = \theta(t)$ of Riemann invariant R^2 one can find

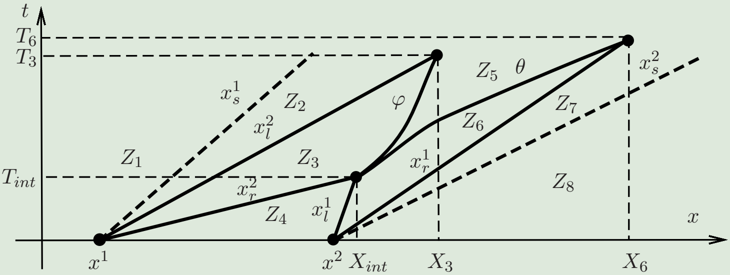
$$(\theta - x^2)^{1/2} = (q^2)^{3/2}\left(t^{1/2} - T_{int}^{1/2}\right) + (X_{int} - x^2)^{1/2}$$

Zone $\mathbb{Z}_3$ disappears at the point (T_3, X_3), when the characteristic $x = \varphi(t)$ intersects the characteristic $x = x_l^2(t)$. From equation $X_3 = \varphi(T_3) = x_l^2(T_3)$ we have

$$T_3 = \frac{(q^2 - q^1)^2}{(q^1 - \mu^2)^2} T_{int}, \quad X_3 = x^1 + q^1\mu^2\mu^2 T_3$$

Zone $\mathbb{Z}_6$ disappears at the point (T_6, X_6), when the characteristic $x = \theta(t)$ intersects the characteristic $x = x_r^1(t)$. From equation $X_6 = \theta(T_6) = x_r^1(T_6)$ we have

$$T_6 = \frac{(q^2 - q^1)^2}{(q^2 - \mu^1)^2} T_{int}, \quad X_6 = x^2 + \mu^1\mu^1 q^2 T_6$$



Zone $\mathbb{Z}_5$

For equations

$$\frac{\partial R^k}{\partial t} + \lambda^k(R^1, R^2)\frac{\partial R^k}{\partial x} = 0, \quad k = 1, 2,$$
$$\lambda^1(R^1, R^2) = R^1 R^1 R^2, \quad \lambda^2(R^1, R^2) = R^2 R^1 R^2$$

we have the Goursat problem with initial data that have weak discontinuities on the characteristics $x = \varphi(t)$, $x = \theta(t)$

$$R^1\big|_{x=\varphi(t)} = q^1, \quad R^2\big|_{x=\varphi(t)} = R^2_a(z^2(\varphi(t), t)),$$

$$R^1\big|_{x=\theta(t)} = R^1_a(z^1(\theta(t), t)), \quad R^2\big|_{x=\theta(t)} = q^2$$

At the point (T_{int}, X_{int})

$$R^1\big|_{t=T_{int}} = q^1, \quad R^2\big|_{t=T_{int}} = q^2$$

The hodograph method

For system

$$\frac{\partial R^k}{\partial t} + \lambda^k(R^1, R^2)\frac{\partial R^k}{\partial x} = 0, \quad k = 1, 2,$$

we can apply the classical hodograph method. Using the replacement of independent and dependent variables $(R^1, R^2) \rightleftharpoons (x, t)$ we get

$$x_{R^2} - \lambda^1 t_{R^2} = 0, \quad x_{R^1} - \lambda^2 t_{R^1} = 0.$$

Using the compatibility conditions we get

$$t_{R^1R^2} + \frac{2}{R^2 - R^1}(t_{R^1} - t_{R^2}) = 0$$

The Riemann-Green function is defined

$$V(r^1, r^2 | R^1, R^2) = \frac{((R^1 + R^2)(r^1 + r^2) - 2(R^1R^2 + r^1r^2))(r^1 - r^2)}{(R^1 - R^2)^3}$$

Expression for $t(R^1, R^2)$

$$t(R^1, R^2) = T_{int} V(q^1, q^2 | R^1, R^2) =$$
$$= \frac{(x^2 - x^1)(2R^1R^2 + 2q^1q^2 - (q^1 + q^2)(R^1 + R^2))}{q^1q^2(R^1 - R^2)^3}$$

The initial condition

$$R^1\big|_{t=T_{int}} = q^1, \quad R^2\big|_{t=T_{int}} = q^2$$

is satisfied

$$t(q^1, q^2) = T_{int} V(q^1, q^2 | q^1, q^2) = T_{int}$$

The equations

$$\frac{\partial R^k}{\partial t} + \lambda^k(R^1, R^2)\frac{\partial R^k}{\partial x} = 0, \quad k = 1, 2,$$

have symmetry property. After a change of variables

$$R^1 = \frac{1}{K^1}, \quad R^2 = \frac{1}{K^2}$$

we get

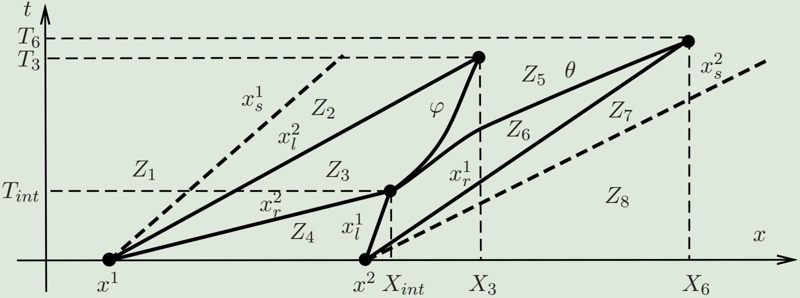
$$x_{K^1K^2} + \frac{2}{K^2 - K^1}(x_{K^1} - x_{K^2}) = 0$$

Expression for $x(R^1, R^2)$

$$x(R^1,R^2) = (x^2 - x^1)(R^1R^2)^2\frac{R^2 + R^1 - 2(q^1 + q^2)}{q^1q^2(R^1 - R^2)^3} +$$

$$+\frac{(x^1(R^1)^3 - x^2(R^2)^3) + 3R^1R^2(R^2x^2 - R^1x^1)}{(R^1 - R^2)^3}$$

Functions $t(R^1, R^2)$, $x(R^1, R^2)$ determine the implicit solution.



Solution on isochrones

Let's fix some moment $t_* \in [T_{int}, \min(T_3, T_6)]$ and consider the level line (isochrone) $t(R^1, R^2) = t_*$.
Differentiating functions $t(R^1, R^2)$, $x(R^1, R^2)$ with respect to x we get

$$0 = t_{R^1} R^1_x + t_{R^2} R^2_x, \quad 1 = x_{R^1} R^1_x + x_{R^2} R^2_x$$

To determine $R^1(x, t)$, $R^2(x, t)$ on isochrones we have the Cauchy problem

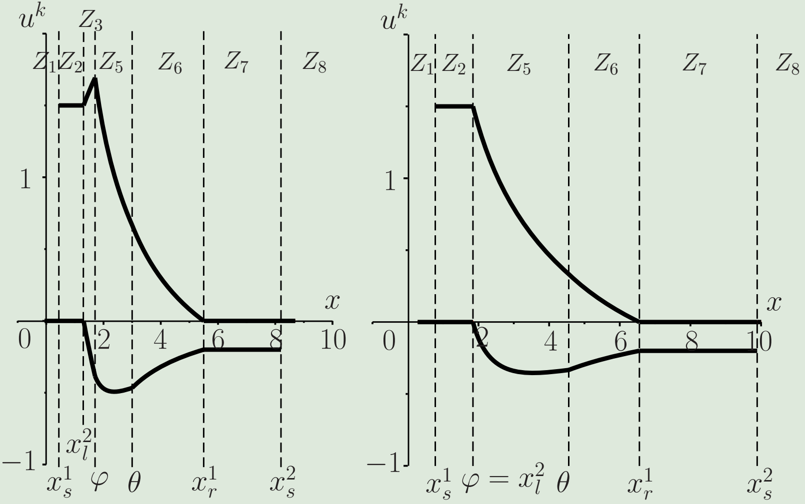
$$\frac{dR^1(x, t_*)}{dx} = -\frac{t_{R^2}(R^1, R^2)}{\Delta(R^1, R^2)}, \quad \frac{dR^2(x, t_*)}{dx} = \frac{t_{R^1}(R^1, R^2)}{\Delta(R^1, R^2)},$$

$$\Delta = t_{R^1} x_{R^2} - t_{R^2} x_{R^1} = (\lambda^1 - \lambda^2) t_{R^1} t_{R^2}$$

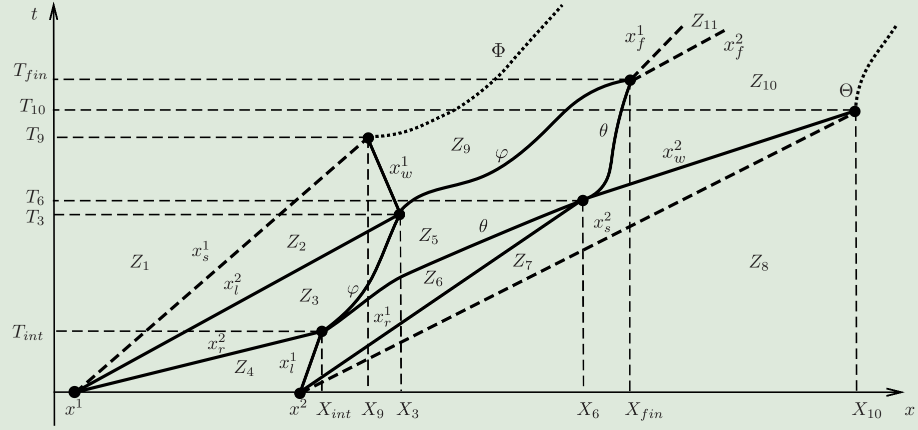
$$R^1(x_*, t_*) = q^1, \quad R^2(x_*, t_*) = R^2_a(x_*, t_*), \quad x_* = \varphi(t_*)$$

Integrating from $\varphi(t_*)$ to $\theta(t_*)$ we obtain the solution at the moment t_* in zone $\mathbb{Z}_5$.

Solution at the moment $t_* = 0.018 > T_{int}$ and $t_* = 1/45 = T_3$



Evolution of initial discontinuities



Evolution of initial discontinuities at the moment $t = +T_3$

In the process of evolution the weak discontinuities cannot disappear and move along the characteristics. The discontinuity of Riemann invariant R^1 moves along the characteristic λ^1, the discontinuity of Riemann invariants R^2 moves along the characteristic λ^2. At the moment $t = T_3$ the Riemann invariants R^1, R^2 have weak discontinuities.

Notations

$R_5^1(x,t)$, $R_5^2(x,t)$ — solution in the zone $\mathbb{Z}_5$
$x = x_w^1(t)$ — lines of weak discontinuity of Riemann invariant R^1
$x = x_w^2(t)$ — lines of weak discontinuity of Riemann invariant R^2
$x = \varphi(t)$ — line of weak discontinuity of Riemann invariant R^2
$x = \theta(t)$ — line of weak discontinuity of Riemann invariant R^1

In the zone $\mathbb{Z}_9$ the Riemann invariants R^2 is constant, $R^2 = \mu^2$. In the zone $\mathbb{Z}_{10}$ the Riemann invariants R^1 is constant, $R^1 = \mu^1$. So in these zones the solution is described by **one hyperbolic equation**. We can use the classical method of characteristics.

Evolution of initial discontinuities at the moment $t = +T_3$

We consider the equation

$$R^1_t + \lambda^1(R^1, \mu_2)R^1_x = 0$$

The continuity condition for R^1, R^2 on the lines $x = x^1_w(t)$, $x = \varphi(t)$

$$R^1\big|_{x=x^1_w(t)} = q^1, \quad R^2\big|_{x=x^1_w(t)} = \mu^2,$$

$$R^1\big|_{x=\varphi(t)} = R^1_5\big|_{x=\varphi(t)}, \quad \mu^2 = R^2_5\big|_{x=\varphi(t)}$$

To find $x^1_w(t)$ we have the Cauchy problem

$$\frac{dx^1_w(t)}{dt} = \lambda^1(q^1, \mu^2), \quad x^1_w(T_3) = X_3$$

The solution is

$$x^1_w(t) = X_3 + q^1 q^1 \mu^2 (t - T_3)$$

Evolution of initial discontinuities at the moment $t = +T_3$

Function $\varphi(t)$

Parametric representation of $\varphi(t)$ is

$$t = t(\rho^1, \mu^2), \quad \varphi(t) = x(\rho^1, \mu^2), \quad q^1 \leqslant \rho^1 \leqslant \mu^1,$$

where ρ^1 is parameter, actually ρ^1 is the value of Riemann invariant R^1 on the line $x = \varphi(t)$

Function $\theta(t)$

Parametric representation of $\theta(t)$ is

$$t = t(\mu^1, \rho^2), \quad \theta(t) = x(\mu^1, \rho^2), \quad \mu^2 \leqslant \rho^2 \leqslant q^2,$$

where ρ^2 is parameter

Function $R^1(x,t)$ in the zone $\mathbb{Z}_9$

Using method of characteristics we have the Cauchy problem

$$\frac{dR^1}{dt} = 0, \quad \frac{dx}{dt} = \lambda^1(R^1,\mu^2), \quad \frac{d}{dt} = \frac{\partial}{\partial t} + \lambda^1(R^1,\mu^2)\frac{\partial}{\partial x},$$

$$R^1\big|_{t=\tau} = R^1_5(\varphi(\tau),\tau), \quad x\big|_{t=\tau} = \varphi(\tau)$$

The solution is

$$R^1(x,t) = R^1_5(\varphi(\tau),\tau), \quad \tau = \tau(x,t),$$

where $\tau(x,t)$ is implicitly defined by the relation

$$x = \varphi(\tau) + R^1_5(\varphi(\tau),\tau)R^1_5(\varphi(\tau),\tau)\mu^2(t-\tau)$$

Applied method

To find $R^1(x,t)$ for any fixed value $t = t_*$ we replace $R^1_5(\varphi(\tau),\tau))$ to parameter ρ^1. Then we find the root of equation

$$t_* = t(\rho^1_*, \mu^2), \quad q^1 \leqslant \rho^1_* \leqslant \mu^1$$

Root ρ^1_* is the value of Riemann invariant which corresponds to intersection of isochrone $t = t_*$ and line $x = \varphi(t)$ in (x,t)–plane.
After changing $R^1_5(\varphi(\tau),\tau) \to \rho^1$ we have parametric representation R^1 on isochrone

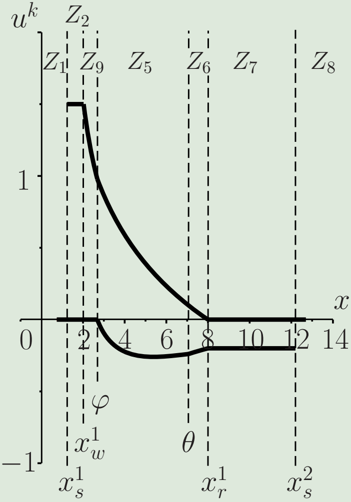
$$R^1(x,t_*) = \rho^1, \quad q^1 \leqslant \rho^1 \leqslant \rho^1_* \leqslant \mu^1,$$

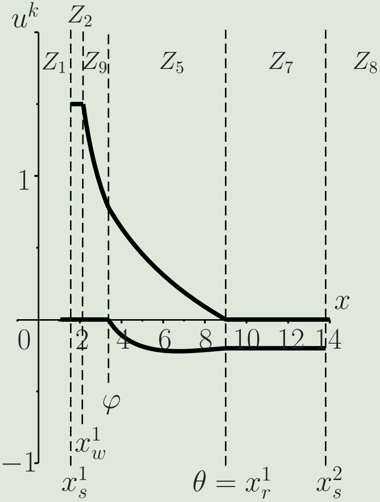
$$x = \varphi(\tau) + \rho^1\rho^1\mu^2(t_* - \tau),$$

where

$$\tau = t(\rho^1, \mu^2), \quad \varphi(\tau) = x(\rho^1, \mu^2)$$

Solution at the moment $t_* = 0.028 > T_3$ and $t_* = 0.032 = T_6$





Function $R^2(x, t)$ in the zone $\mathbb{Z}_{10}$

Similarly the problem is solved in the neighborhood of point (X_6, T_6). To write the solution it is enough to replace indices $1 \leftrightarrows 2$, $\varphi \to \theta$ and change the intervals of parameter

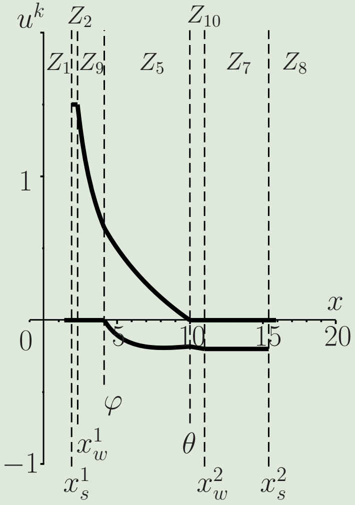
$$R^2(x, t_*) = \rho^2, \quad \mu^2 \leqslant \rho^2 \leqslant \rho_*^2 \leqslant q^2,$$

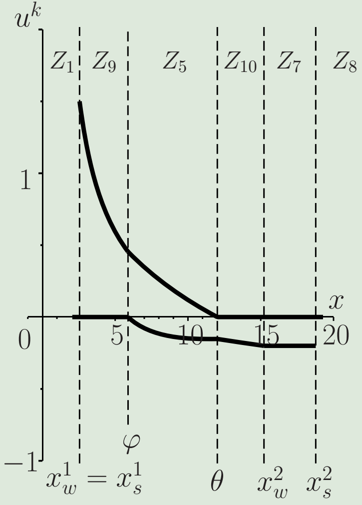
$$t_* = t(\mu^1, \rho_*^2), \quad \mu^2 \leqslant \rho_*^2 \leqslant q^2,$$

$$x = \theta(\tau) + \rho^2\rho^2\mu^1(t_* - \tau),$$

$$\tau = t(\mu^1, \rho^2), \quad \theta(\tau) = x(\mu^1, \rho^2)$$

Solution at the moment $t_* = 0.036 > T_6$ and $t_* = 2/45 = T_9$





At the moment $t = T_9$ line $x = x_w^1(t)$ intersects line $x = x_s^1(t)$. Point (X_9, T_9) is

$$T_9 = \frac{\mu^2 - q^1}{\mu^1 - q^1} T_3, \quad X_9 = x^1 + q^1 \mu^1 \mu^2 T_9$$

From moment $t = T_9$ the left border of zone $\mathbb{Z}_9$ is changed. The Riemann invariant R^2 is constant, $R^2 = \mu^2$, so one of the Rankine-Hugoniot conditions is automatically satisfied, and another condition has the form

$$\frac{D}{\mu^2} \left[\frac{1}{R^1} \right] = - \left[R^1 \right]$$

Evolution of initial discontinuities at the moment $t = +T_9$

On new border $x = \Phi(t)$ of zone $\mathbb{Z}_9$ we have

$$R^1(\Phi(t) - 0, t) = \mu^1, \quad R^1(\Phi(t) + 0, t) = R_9^1(\Phi(t) + 0, t),$$

$R_9^1(x, t)$ is Riemann invariant in zone $\mathbb{Z}_9$

$$R_9^1(x, t) = R_5^1(\varphi(\tau), \tau), \quad \tau = \tau(x, t),$$

where $\tau = \tau(x, t)$ is implicitly determined by the relation

$$x = \varphi(\tau) + R_5^1(\varphi(\tau), \tau) R_5^1(\varphi(\tau), \tau) \mu^2 (t - \tau)$$

Notations

$$\rho^1(t) = R^1(\Phi(t) + 0, t) = R_9^1(\Phi(t) + 0, t)$$

After substitution the Rankine-Hugoniot condition is

$$\frac{d\Phi(\beta)}{d\beta} = D = \mu^1 \mu^2 \rho^1(\beta),$$

$$\Phi(\beta) = \varphi(\tau) + \mu^2 \rho^1(\beta) \rho^1(\beta)(\beta - \tau),$$

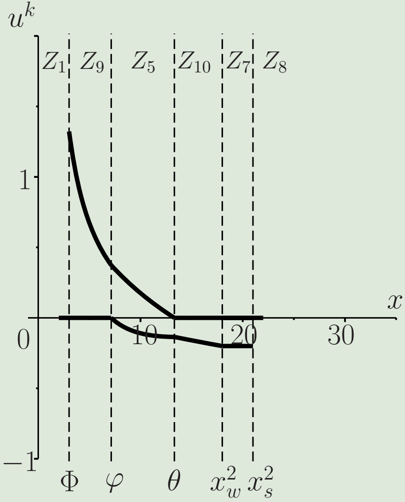
$$\tau = t(\rho^1(\beta), \mu^2), \quad \varphi(\tau) = x(\rho^1(\beta), \mu^2)$$

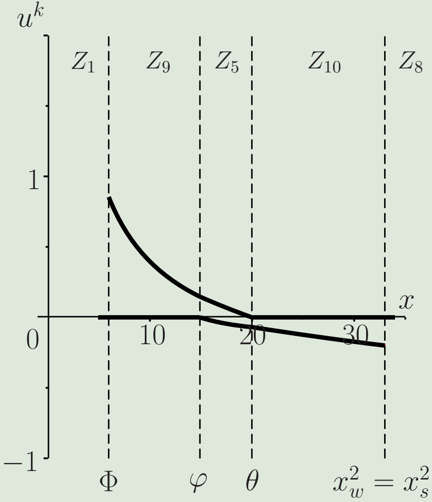
In fact β is the current time. Initial conditions are

$$\rho^1(T_9) = q^1, \quad \Phi(T_9) = X_9$$

Evolution of initial discontinuities at the moment $t = +T_9$

Solution at the moment $t_* = 0.05 > T_9$ and $t_* = 0.08 = T_{10}$





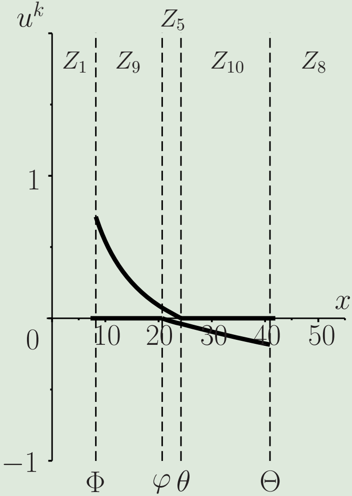
Evolution of initial discontinuities at the moment $t = +T_{10}$

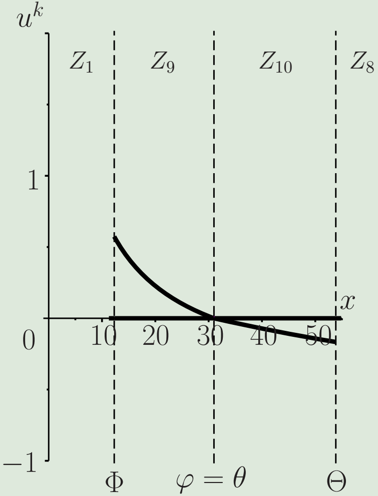
Similarly, (X_{10}, T_{10}) is the point of interaction between weak and strong discontinuities R^2

$$T_{10} = \frac{\mu^1 - q^2}{\mu^2 - q^2} T_6, \quad X_{10} = x^2 + q^2 \mu^1 \mu^2 T_{10}$$

To get the solution we need to change $\Phi \to \Theta$, $1 \rightleftharpoons 2$.

Solution at the moment $t_* = 0.1 > T_{10}$ and $t_* = 2/15 = T_{fin}$





Evolution of initial discontinuities at the moment $t = +T_{fin}$

Point (X_{fin}, T_{fin}) is the point of mixture separation

$$T_{fin} = T_{int} V(q^1, q^2 | \mu^1, \mu^2) = t(\mu^1, \mu^2), \quad X_{fin} = x(\mu^1, \mu^2)$$

New zone $\mathbb{Z}_{11}$ appears ($R^1 = \mu^1$, $R^2 = \mu^2$ and $u^1 = u^2 = 0$)

$$\mathbb{Z}_{11} = \{(\mu^1, \mu^2), (x_f^1(t), x_f^2(t))\},$$

$$x_f^1 = X_{fin} + \mu^1 \mu^1 \mu^2 (t - T_{fin}), \quad x_f^2 = X_{fin} + \mu^2 \mu^1 \mu^2 (t - T_{fin})$$

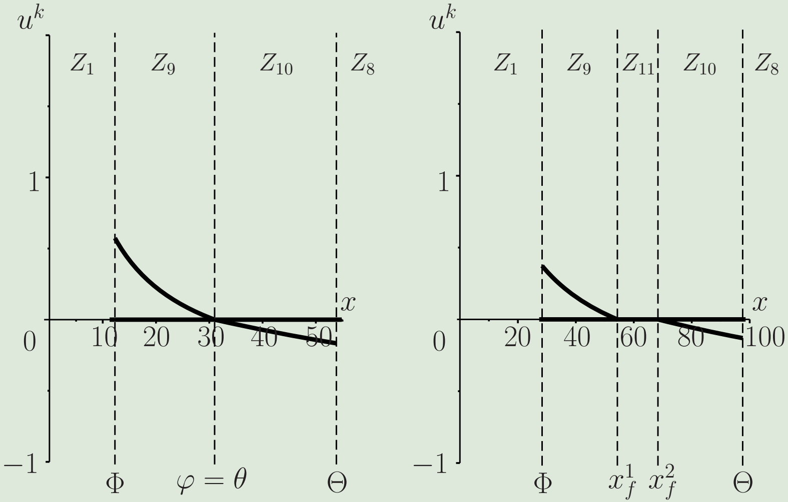
New borders of zones $\mathbb{Z}_9$ and $\mathbb{Z}_{10}$ are

$$\mathbb{Z}_9 = \{(R^1(x,t), \mu^2), (\Phi(t), x_f^1(t))\},$$

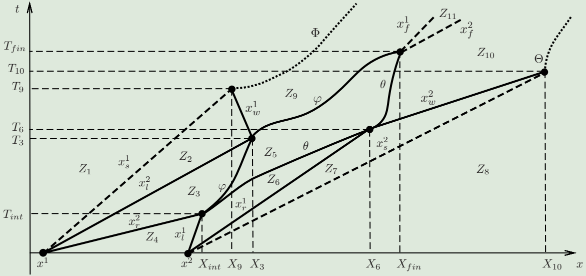
$$\mathbb{Z}_{10} = \{(\mu^1, R^2(x,t)), (x_f^2(t), \Theta(t))\}$$

Evolution of initial discontinuities at the moment $t = +T_{fin}$

Solution at the moment $t_* = 2/15 = T_{fin}$, $t_* = 0.25 > T_{fin}$



- We got full picture of the two component mixture separation. For any point on (x,t)–plane we can find the concentrations.
- Proposed method is effective in all cases when the Riemann-Green function is defined
- The method proposed for recovery of an explicit solution with the help of its implicit form
- This method allows not only to solve the Goursat problem, but also to solve effectively the Cauchy problem with arbitrary initial data.



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Thank you for your attention!