Surface and boundary phenomenon

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Technical Note

An introduction to the derivation of surface balance equations without the excruciating pain

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A R T I C L E   I N F O

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A B S T R A C T

Analyzing complex fluid flow problems that involve multiple coupled domains, each with their respective set of governing equations, is not a trivial undertaking. Even more complicated is the elaborate and tedious task of specifying the interface and boundary conditions between various domains. This paper provides an elegant, straightforward and universal method that considers the nature of those shared boundaries and derives the appropriate conditions at the interface, irrespective of the governing equations being solved. As a first example, a well-known interface condition is derived using this method. For a second example, the set of boundary conditions necessary to solve a baseline aerothermodynamics coupled plain/porous flow problem is derived. Finally, the method is applied to two more flow configurations, one consisting of an impermeable adiabatic wall and the other an ablating surface.

Boundary condition

- Arguably, the boundary conditions are the most difficult thing to set (and understand) when designing (or using) a numerical modeling code (CFD or MR)
- Even more difficult when comes the time to couple two codes
- Current approach is to solve “given” equation that will set the properties at the wall
- For instance, for a fluid flowing parallel to a porous surface, the “coupling” equation is the so-called Beavers-Joseph boundary condition, which was obtained experimentally:

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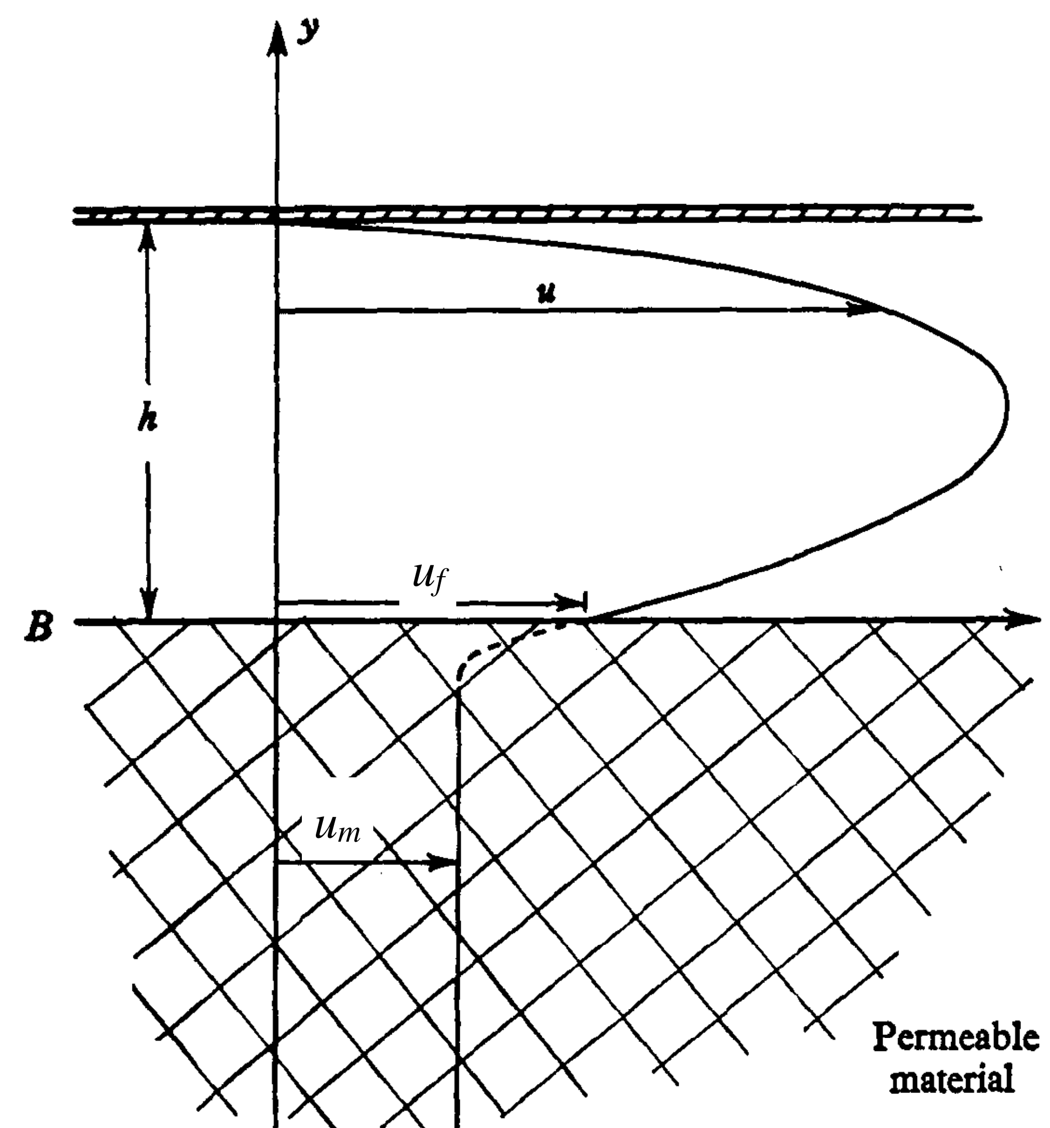

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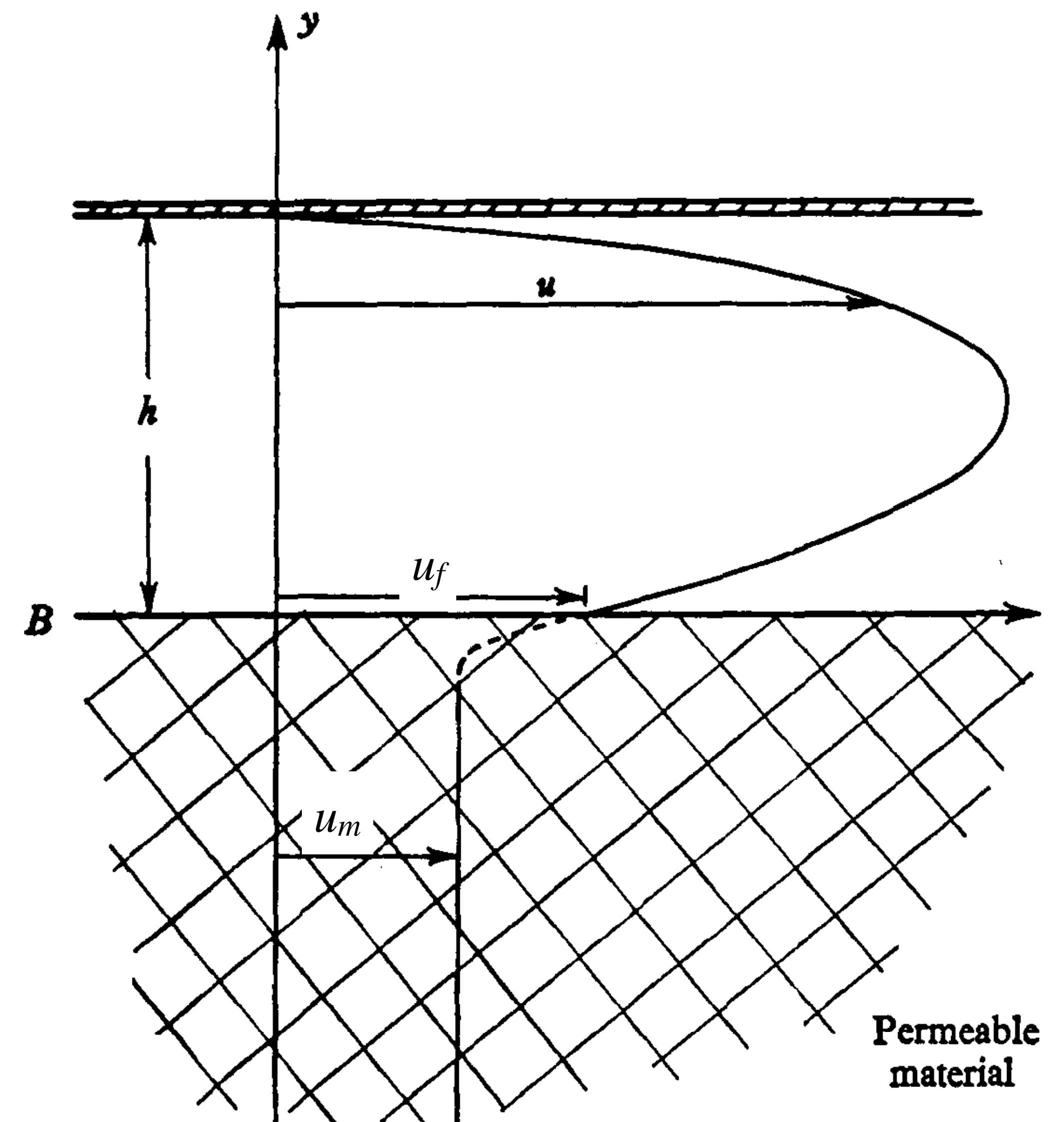
Beavers-Joseph (1967)



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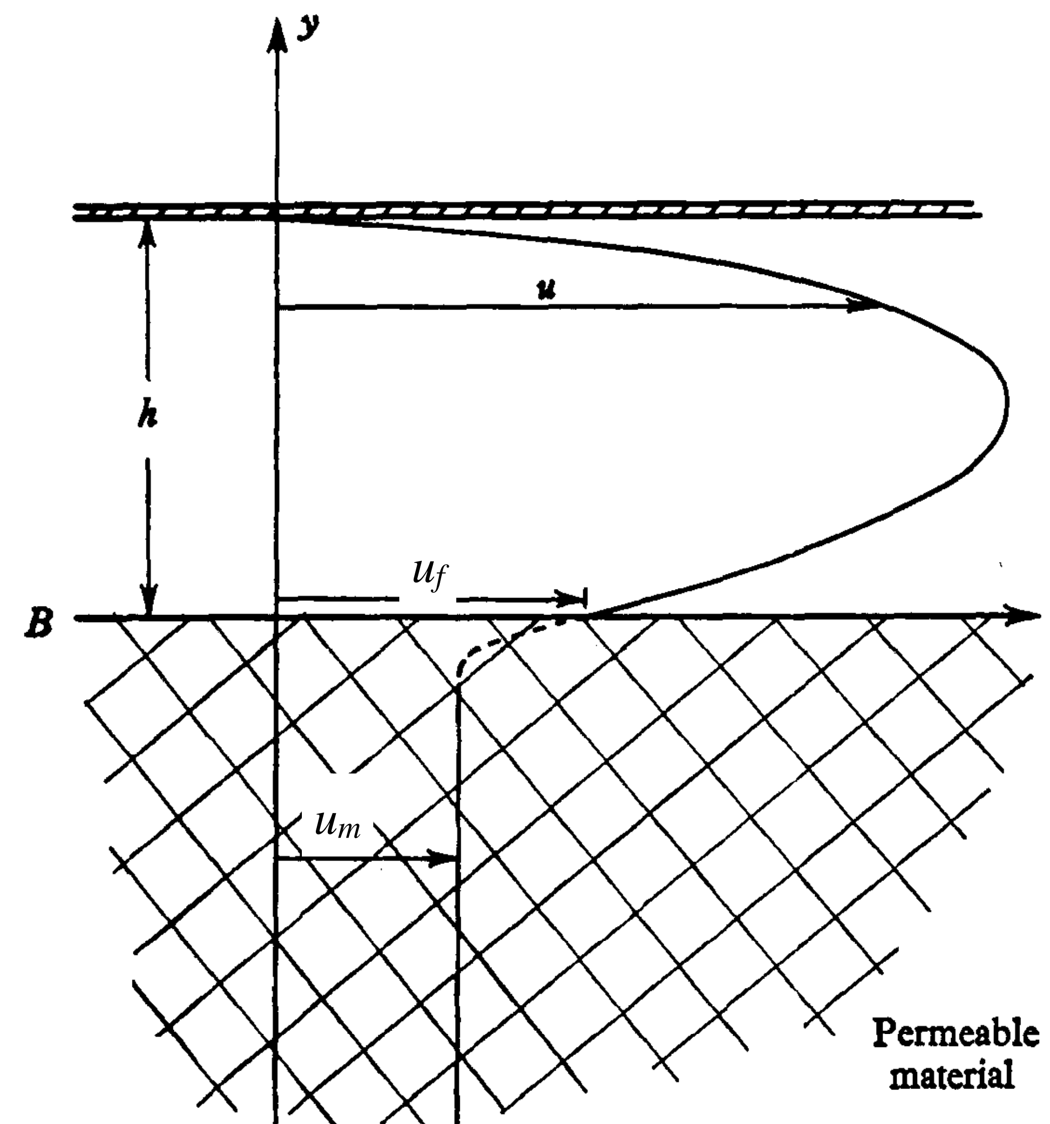

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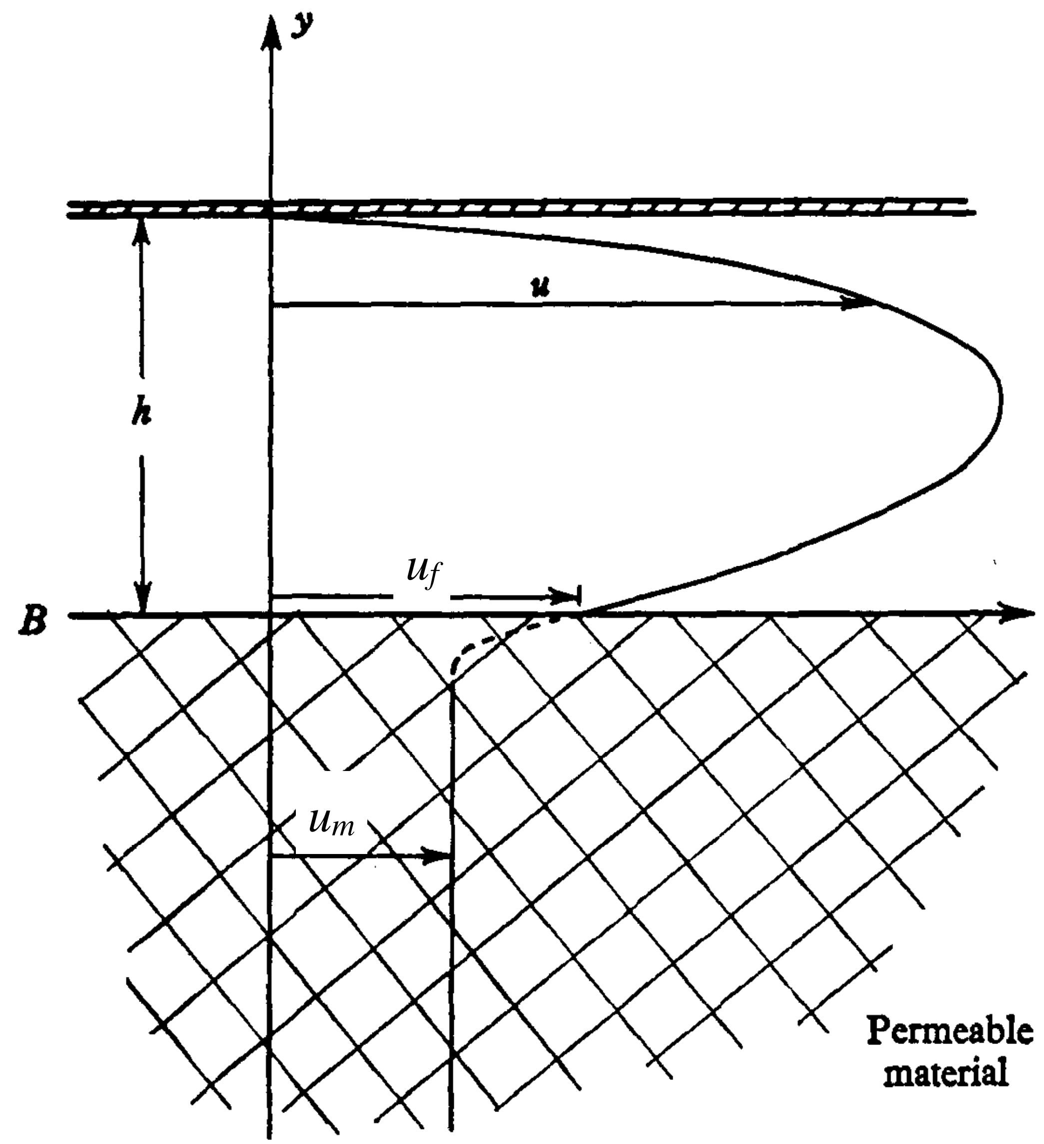
$$\frac{\partial u_f}{\partial y} + \frac{\partial v_f}{\partial x} = \frac{\alpha_{BJ}}{K^{1/2}}(u_f - u_m)$$ Jones (1973)



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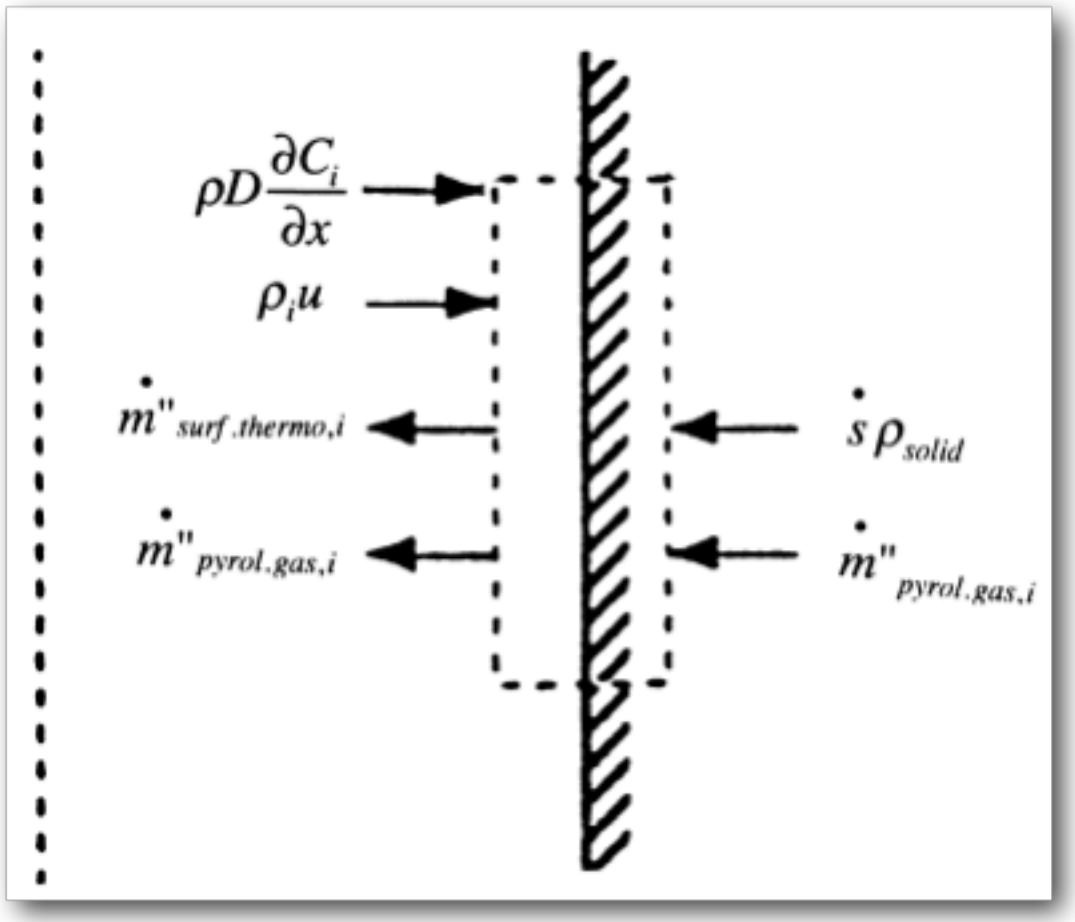
Boundary Conditions

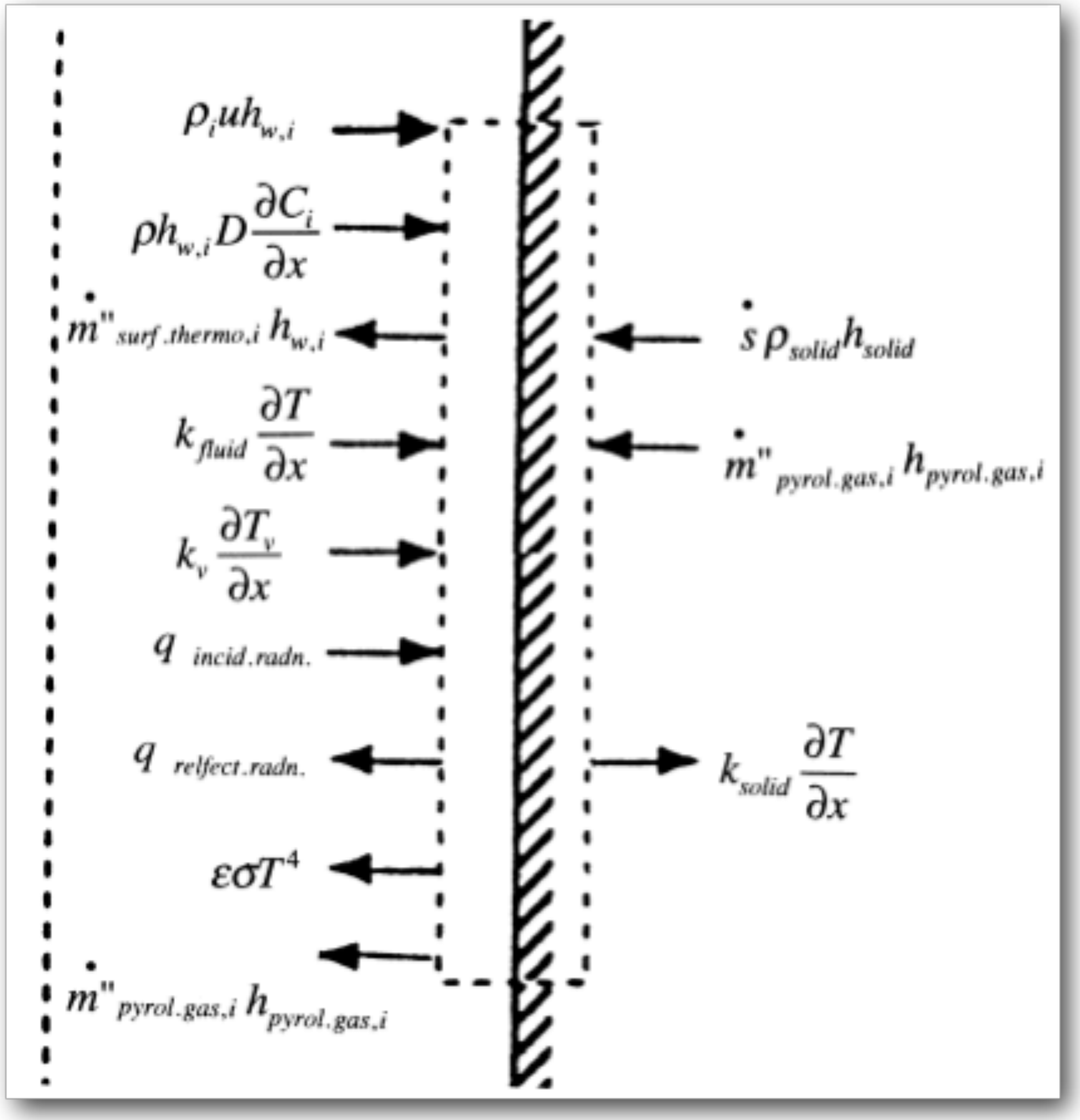
- When coupling, the state-of-the-art practice is to solve the Surface Balance Equation (mass and energy)

Surface Mass Balance (SMB)



Havstad (2001)

Surface Energy Balance (SEB)



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Boundary Conditions

JOURNAL OF THERMOPHYSICS AND HEAT TRANSFER
Vol. 8, No. 1, Jan.–March 1994

Review of Numerical Procedures for Computational Surface Thermochemistry

Frank S. Milos* and Daniel J. Rasky†
NASA Ames Research Center, Moffett Field, California 94035

Models and equations for surface thermochemistry and near-surface thermophysics of aerodynamically heated thermal protection materials are reviewed, with particular emphasis on computational boundary conditions for surface mass and energy transfer. The surface energy and mass balances, coupled with an appropriate ablation or surface catalysis model, provide complete thermochemical boundary conditions for a true multidisciplinary solution of the fully coupled fluid-dynamics/solid mechanics problem. Practical approximate solutions can be obtained by using a detailed model with full thermophysics for either the solid or fluid phase and a semianalytic method for the other half of the problem. A significant increase in the state-of-the-art in aerothermal computational fluid dynamics is possible by uniting computational fluid dynamic (CFD) methodology with surface thermochemistry boundary conditions and the heat-balance-integral method.

Boundary Conditions

- The Surface Energy Balance (SEB) equation

Flow field = Material

Nonequilibrium flow, material conductivity, ablation

$$k_T \frac{\partial T}{\partial \eta} + k_V \frac{\partial T_V}{\partial \eta} + \sum_{i=1}^{N_c} \rho h_i D \frac{\partial y_i}{\partial \eta} = q_{\text{cond}} + \dot{m}_{sw}(h_w - h_{sw})$$

Nonequilibrium flow, radiative surface, incident radiation, material conductivity, ablation

$$k_T \frac{\partial T}{\partial \eta} + k_V \frac{\partial T_V}{\partial \eta} + \sum_{i=1}^{N_c} \rho h_i D \frac{\partial y_i}{\partial \eta} + q_r = (1 - \alpha_{sw})q_r + F\sigma\epsilon_{sw}T_w^4 + q_{\text{cond}} + \dot{m}_{sw}(h_w - h_{sw})$$

Convective approximation, material conductivity, ablation

$$\rho_e u_e C_h(h_r - h_w) + q_r = (1 - \alpha_{sw})q_r + F\sigma\epsilon_{sw}T_w^4 + q_{\text{cond}} + \dot{m}_{sw}(h_w - h_{sw})$$

Milos, F. S. and Rasky, D., "Review of numerical procedures for computational surface thermochemistry," Journal of Thermophysics and Heat Transfer, Vol. 8, No. 1, Jan 1994, pp. 24–34.

Boundary Conditions

- The Surface Mass Balance (SMB) equation

Flow field = Material

Surface ablation, chemical non equilibrium (species conservation)

$$\rho D \frac{\partial y_i}{\partial \eta} = \sum_{k=1}^{N_r} \nu_{ki} r_k M_i + \dot{m}_{sw}(y_i - Y_{swi}), \qquad i = 1, N_c$$

Surface ablation, chemical equilibrium (element conservation)

$$\rho D \frac{\partial \tilde{y}_k}{\partial \eta} = \dot{m}_{sw}(\tilde{y}_k - \tilde{y}_{swk}), \qquad k = 1, N_{el}$$

Surface ablation and pyrolysis, chemical equilibrium

$$\rho D \frac{\partial \tilde{y}_k}{\partial \eta} = (\dot{m}_{cw} + \dot{m}_{gw})\tilde{y}_k - \dot{m}_{cw}\tilde{y}_{cwk} - \dot{m}_{gw}\tilde{y}_{gwk}$$

Milos, F. S. and Rasky, D., “Review of numerical procedures for computational surface thermochemistry,” Journal of Thermophysics and Heat Transfer, Vol. 8, No. 1, Jan 1994, pp. 24–34.

Boundary Conditions

- Energy and mass are used… but what about momentum?
- If the material response code is only solving energy and mass (CMA, "old" FIAT, etc.), then no need to do so
- However, modern material response code solve for momentum (Darcy's Law, Brinkman equation, etc.)
- Simple solution is to use equal pressure at the wall (zero pressure gradient in the normal direction)

$$p_{nc} = p_w$$

- But the velocity is not zero at the wall… so dynamic pressure can be included

$$p_{nc} + \rho_{nc} v_{nc}^2 = p_w(\rho_w, T_w) + \rho_w v_w^2$$

- This can be solved to obtain wall properties… however, this neglects various terms, such as skin friction…

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Reynolds Transport Theorem

- This require a lot of work, and an intimate understanding of the surface
- But more importantly, it is confusing (and <u>excruciatingly</u> painful to apply)
- Why not, instead, let the two codes figure it out: after all, the main tasks of all codes are to calculate fluxes…
- Conservation equations can be written in the form of the Reynolds Transport Theorem (RTT)

$$\int_V \frac{\partial \mathbf{Q}}{\partial t}\, dV + \oint_A \mathbf{Q}(\mathbf{u}\cdot\mathbf{n})\, dA = \int_V \mathbf{S}\, dV$$

- The RTT expresses mathematically “common sense”: in a control volume, the time variation of a given quantity is equal to the change of that quantity in the volume (source term) and the net amount of that quantity leaving or entering the volume (surface fluxes)

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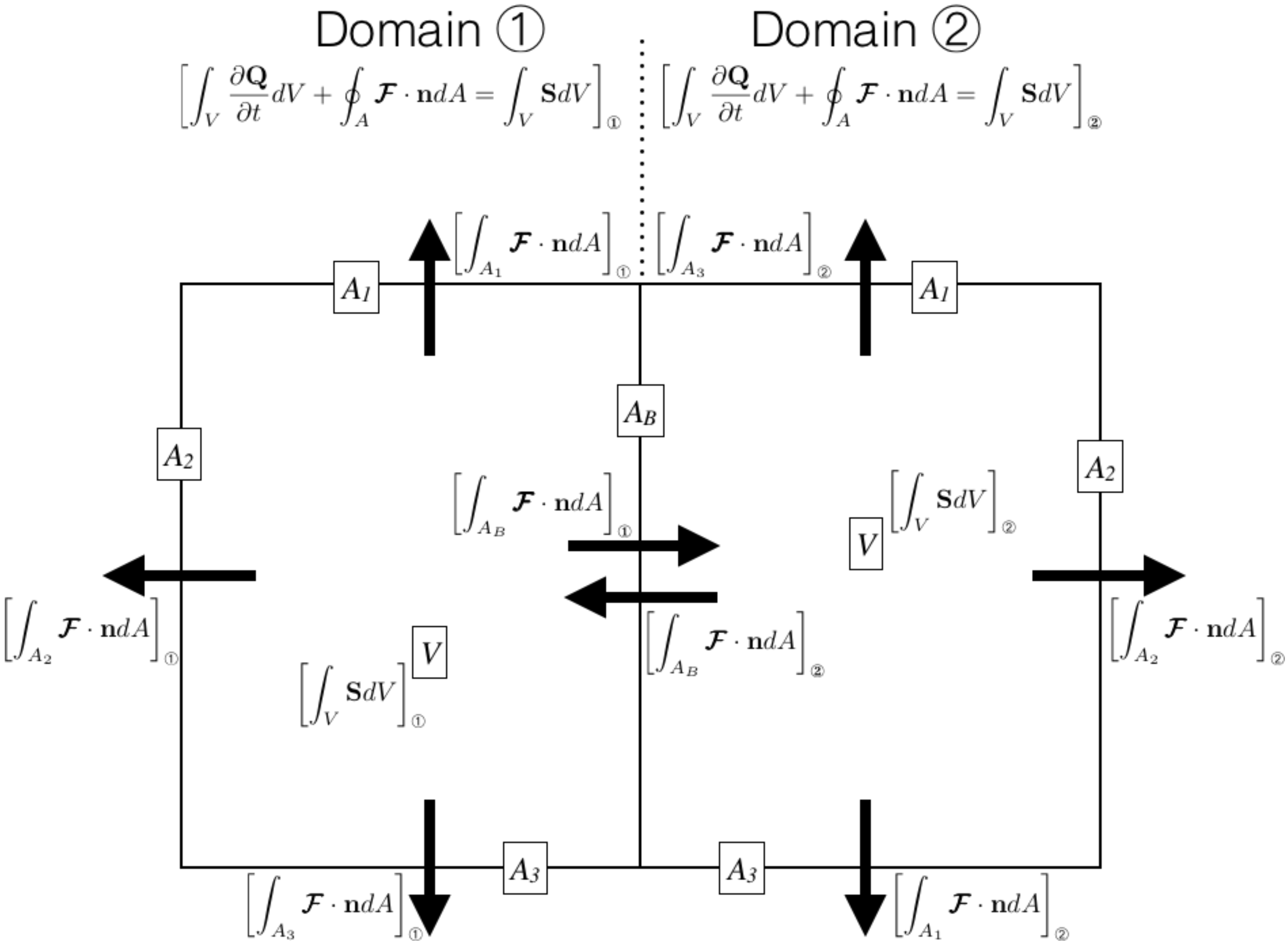
Domains


Domain ①
Domain ②
$\left[\int_V \frac{\partial \mathbf{Q}}{\partial t} dV + \oint_A \boldsymbol{\mathcal{F}} \cdot \mathbf{n} dA = \int_V \mathbf{S} dV\right]_{①}$
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$\left[\int_{A_1} \boldsymbol{\mathcal{F}} \cdot \mathbf{n} dA\right]_{①}$
$\left[\int_{A_3} \boldsymbol{\mathcal{F}} \cdot \mathbf{n} dA\right]_{②}$
A_1
A_1
A_B
A_2
A_2
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V
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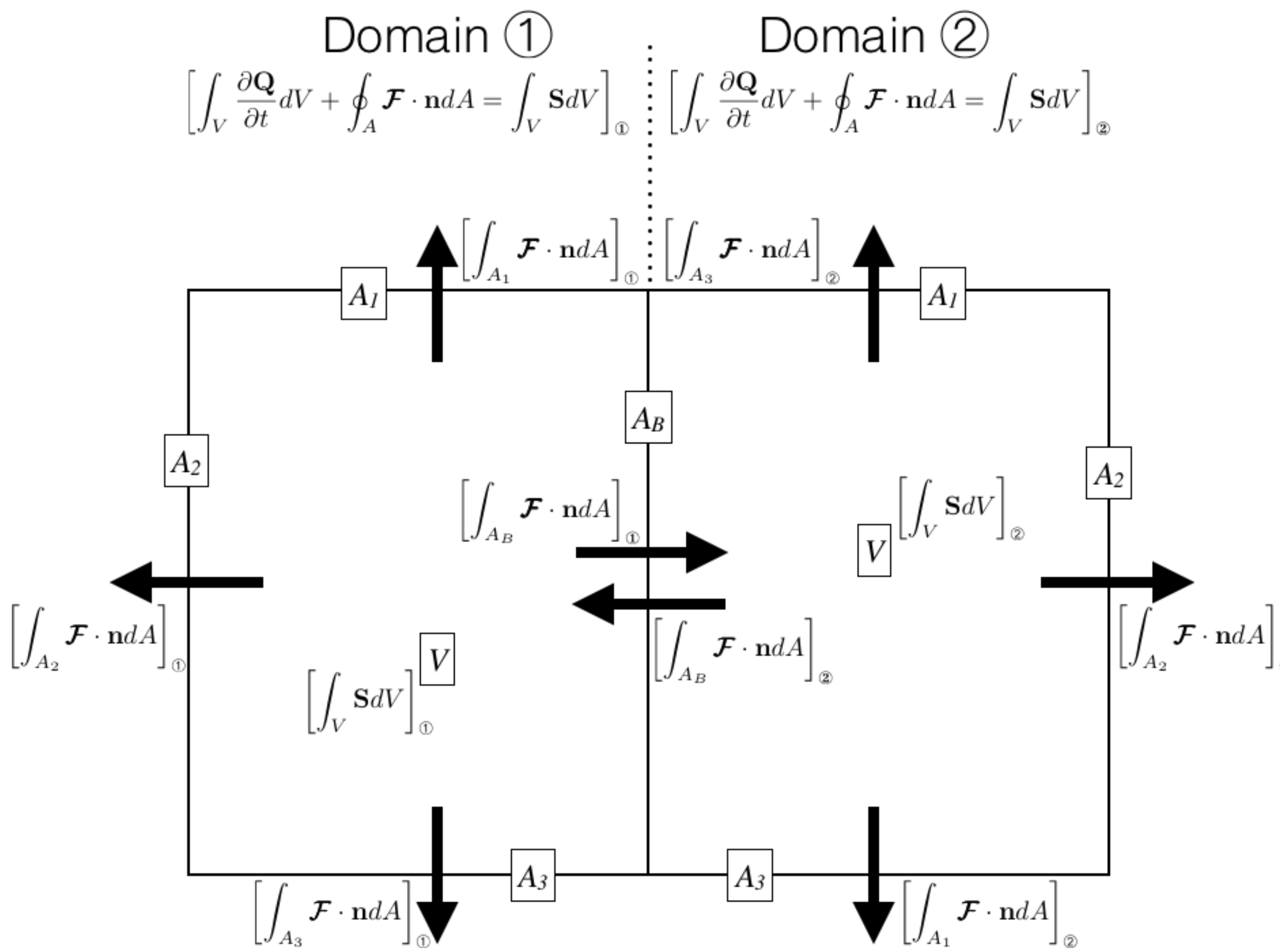
1. Impermeable adiabatic wall

- From this concept, it is also very easy to understand boundary conditions.
- For a solid, adiabatic wall, for instance, all fluxes need to be zero.
  - The boundary condition at the wall is then set so that a net mass, momentum and heat flux of zero is imposed



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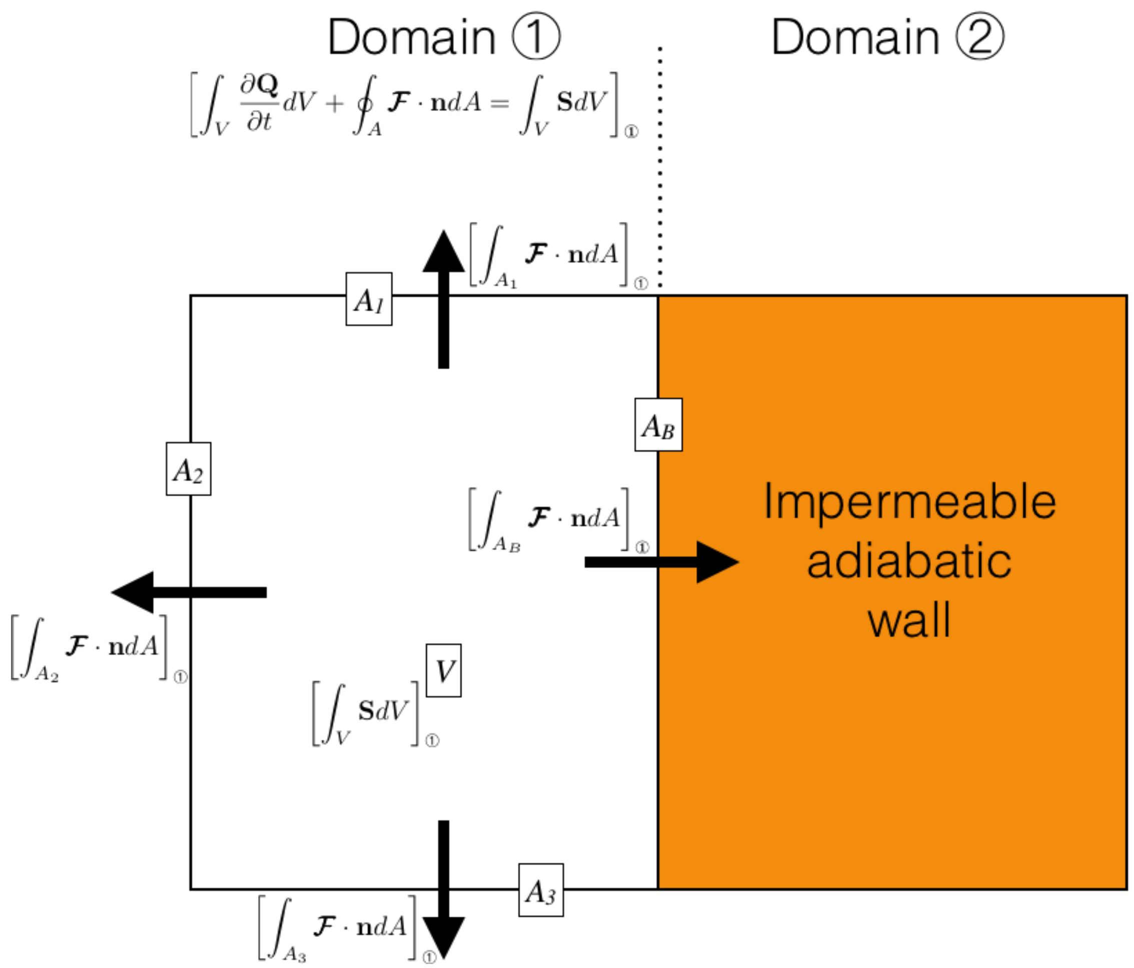

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Flux matching — Wall

Advective fluxes | Diffusive fluxes

Flow field

$$\mathbf{F} = \begin{pmatrix} \rho_1 u & \rho_1 v & \rho_1 w \\ \vdots & \vdots & \vdots \\ \rho_{ngs} u & \rho_{ngs} v & \rho_{ngs} w \\ \rho_g u^2 + p & \rho_g vu & \rho_g wu \\ \rho_g uv & \rho_g v^2 + p & \rho_g wv \\ \rho_g uw & \rho_g vw & \rho_g w^2 + p \\ (E+p)u & (E+p)v & (E+p)w \end{pmatrix}, \quad \mathbf{F_d} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{ngs} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \mathbf{q} - \sum_{i=1}^{ngs} (\mathbf{J}_i h_i) & \end{pmatrix}.$$

Material

$$\mathbf{F} = \begin{pmatrix} 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbf{F_d} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}.$$

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Surface balance equations — Wall

- Therefore, the fluxes simply need to be evaluated at the same surface, using the contribution from both sides

$$\left[\int_{A_B} \mathcal{F} \cdot \mathbf{n}\, dA\right]_{①} = \left[\int_{A_B} \mathcal{F} \cdot \mathbf{n}\, dA\right]_{②} + \int_{A_B} \mathbf{S_A}\, dA$$

- Assuming that the surface is perpendicular to *x-dir* the following are obtained

Mass $$\left[\rho_g u\right]_f = 0$$

Momentum $$\left[\rho_g u^2 + p - \tau_{xx}\right]_f = R''_x$$

$$\left[\rho_g u v - \tau_{yx}\right]_f = R''_y$$

$$\left[\rho_g u w - \tau_{zx}\right]_f = R''_z$$

Energy $$\left[\rho_g u h - (\tau_{xx} u + \tau_{xy} v + \tau_{xz} w) + \dot{q}''_x\right]_f = 0$$

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Mass $\cancel{\left[\rho_g u\right]_f = 0}$

Momentum $\left[\cancel{\rho_g u^2} + p - \tau_{xx}\right]_f = R''_x$

$$\left[\cancel{\rho_g uv} - \tau_{yx}\right]_f = R''_y$$

$$\left[\cancel{\rho_g uw} - \tau_{zx}\right]_f = R''_z$$

Energy $\left[\cancel{\rho_g uh} - (\cancel{\tau_{xx} u} + \tau_{xy} v + \tau_{xz} w) + \dot{q}''_x\right]_f = 0$

[1] Martin, A., Zhang, H., and Tagavi, K. A., “An introduction to a systematic derivation of surface balance equations without the excruciating pain,” Int. J. of Heat and Mass Transfer, Vol. 115, Part A, December 2017, pp. 992–999.

Surface balance equations — Wall

- Therefore, the fluxes simply need to be evaluated at the same surface, using the contribution from both sides

$$\left[\int_{A_B} \mathcal{F}\cdot\mathbf{n}\,dA\right]_{①} = \left[\int_{A_B} \mathcal{F}\cdot\mathbf{n}\,dA\right]_{②} + \int_{A_B} \mathbf{S_A}\,dA$$

- Assuming that the surface is perpendicular to *x-dir* the following are obtained
  - Solving
  - Assuming non-slip condition

Mass $\cancel{\left[\rho_g u\right]_f = 0}$

Momentum $\left[\cancel{\rho_g u^2} + p - \tau_{xx}\right]_f = R''_x$

$\left[\cancel{\rho_g u v} - \tau_{yx}\right]_f = R''_y$

$\left[\cancel{\rho_g u w} - \tau_{zx}\right]_f = R''_z$

Energy $\left[\cancel{\rho_g u h} - (\cancel{\tau_{xx} u} + \cancel{\tau_{xy} v} + \cancel{\tau_{xz} w}) + \dot{q}''_x\right]_f = 0$

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$$\left[\int_{A_B} \mathcal{F} \cdot \mathbf{n}\, dA\right]_{①} = \left[\int_{A_B} \mathcal{F} \cdot \mathbf{n}\, dA\right]_{②} + \int_{A_B} \mathbf{S_A}\, dA$$

- Assuming that the surface is perpendicular to *x-dir* the following are obtained

Momentum

$$[p - \tau_{xx}]_f = R''_x$$

$$[-\tau_{yx}]_f = R''_y$$

$$[-\tau_{zx}]_f = R''_z$$

Energy

$$[\dot{q}''_x]_f \equiv \left[-k\frac{\partial T}{\partial x}\right]_f = 0$$

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2. Non-pyrolyzing ablating wall

- The technique can also be applied to derive the equation of an non-pyrolyzing ablating wall
- To do so, a grid advection term (ALE) is added

Flow field

$$\mathcal{F}_{\text{adv}} = \begin{pmatrix} \rho_{g_1} u & \rho_{g_1} v & \rho_{g_1} w \\ \vdots & \vdots & \vdots \\ \rho_{g_{\text{ngs}}} u & \rho_{g_{\text{ngs}}} v & \rho_{g_{\text{ngs}}} w \\ \rho_g u^2 + p & \rho_g uv & \rho_g uw \\ \rho_g vu & \rho_g v^2 + p & \rho_g vw \\ \rho_g wu & \rho_g wv & \rho_g w^2 + p \\ \rho_g hu & \rho_g hv & \rho_g hw \end{pmatrix} \quad \mathcal{F}_{\text{diff}} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{\text{ngs}} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \dot{\mathbf{q}}'' - \sum_{i=1}^{\text{ngs}} (\mathbf{J}_i h_i) & \end{pmatrix} \quad \mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{g_1} u_g & \rho_{g_1} v_g & \rho_{g_1} w_g \\ \vdots & \vdots & \vdots \\ \rho_{g_{\text{ngs}}} u_g & \rho_{g_{\text{ngs}}} v_g & \rho_{g_{\text{ngs}}} w_g \\ \rho_g u u_g & \rho_g v u_g & \rho_g w u_g \\ \rho_g u v_g & \rho_g v v_g & \rho_g w v_g \\ \rho_g u w_g & \rho_g v w_g & \rho_g w w_g \\ \rho_g e u_g & \rho_g e v_g & \rho_g e w_g \end{pmatrix}$$

Material

$$\mathcal{F}_{\text{adv}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \quad \mathcal{F}_{\text{diff}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ -\dot{\mathbf{q}}'' \end{pmatrix} \quad \mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{s1} u_g & \rho_{s1} v_g & \rho_{s1} w_g \\ & \vdots & \\ \rho_{s\text{ngs}} u_g & \rho_{s\text{ngs}} v_g & \rho_{s\text{ngs}} w_g \\ & \mathbf{0} & \\ & \mathbf{0} & \\ & \mathbf{0} & \\ \rho_s e_s u_g & \rho_s e_s v_g & \rho_s e_s w_g \end{pmatrix}$$

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Material

$$\mathcal{F}_{\text{adv}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \quad \text{Mass} \quad \mathcal{F}_{\text{diff}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ -\dot{\mathbf{q}}'' \end{pmatrix} \quad \mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{s1} u_g & \rho_{s1} v_g & \rho_{s1} w_g \\ & \vdots & \\ \rho_{s\text{ngs}} u_g & \rho_{s\text{ngs}} v_g & \rho_{s\text{ngs}} w_g \\ & \mathbf{0} & \\ & \mathbf{0} & \\ & \mathbf{0} & \\ \rho_s e_s u_g & \rho_s e_s v_g & \rho_s e_s w_g \end{pmatrix}$$

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Mass

$$\mathcal{F}_{\text{diff}} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{\text{ngs}} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \dot{\mathbf{q}}'' - \sum_{i=1}^{\text{ngs}} (\mathbf{J}_i h_i) & \end{pmatrix}$$

Momentum

$$\mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{g_1} u_g & \rho_{g_1} v_g & \rho_{g_1} w_g \\ \vdots & \vdots & \vdots \\ \rho_{g_{\text{ngs}}} u_g & \rho_{g_{\text{ngs}}} v_g & \rho_{g_{\text{ngs}}} w_g \\ \rho_g u u_g & \rho_g v u_g & \rho_g w u_g \\ \rho_g u v_g & \rho_g v v_g & \rho_g w v_g \\ \rho_g u w_g & \rho_g v w_g & \rho_g w w_g \\ \rho_g e u_g & \rho_g e v_g & \rho_g e w_g \end{pmatrix}$$

Material

$$\mathcal{F}_{\text{adv}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix}$$

Mass

Momentum

$$\mathcal{F}_{\text{diff}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ -\dot{\mathbf{q}}'' \end{pmatrix}$$

$$\mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{s1} u_g & \rho_{s1} v_g & \rho_{s1} w_g \\ & \vdots & \\ \rho_{s\text{ngs}} u_g & \rho_{s\text{ngs}} v_g & \rho_{s\text{ngs}} w_g \\ & \mathbf{0} & \\ & \mathbf{0} & \\ & \mathbf{0} & \\ \rho_s e_s u_g & \rho_s e_s v_g & \rho_s e_s w_g \end{pmatrix}$$

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Mass

Momentum

Energy

Material

$$\mathcal{F}_{\text{adv}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} \quad \mathcal{F}_{\text{diff}} = \begin{pmatrix} \mathbf{0} \\ \vdots \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{0} \\ -\dot{\mathbf{q}}'' \end{pmatrix} \quad \mathcal{F}_{\text{grid}} = \begin{pmatrix} \rho_{s1} u_g & \rho_{s1} v_g & \rho_{s1} w_g \\ & \vdots & \\ \rho_{\text{sngs}} u_g & \rho_{\text{sngs}} v_g & \rho_{\text{sngs}} w_g \\ & \mathbf{0} & \\ & \mathbf{0} & \\ & \mathbf{0} & \\ \rho_s e_s u_g & \rho_s e_s v_g & \rho_s e_s w_g \end{pmatrix}$$

Mass

Momentum

Energy

Surface balance equations — Ablating wall

Mass $\left[\rho_{g_i}(u - u_g) + J_{x,i}\right]_f = \left[-\rho_i u_g\right]_s$

Momentum $\left[\rho_g u(u - u_g) + p - \tau_{xx}\right]_f = R''_x$

$$\left[\rho_g v(u - u_g) - \tau_{yx}\right]_f = R''_y$$

$$\left[\rho_g w(u - u_g) - \tau_{zx}\right]_f = R''_z$$

Energy $\left[\rho_g(uh - u_g e) - (\tau_{xx}u + \tau_{xy}v + \tau_{xz}w) + \dot{q}''_x + \sum J_{x,i}h_i\right]_f = \left[-\rho_s u_g e_s + \dot{q}''_x\right]_s$

Surface balance equations — Ablating wall

Mass $\left[\rho_{g_i}(\cancel{u}-u_g)+J_{x,i}\right]_f=\left[-\rho_i u_g\right]_s$

Momentum $\left[\cancel{\rho_g u(u-u_g)}+p-\tau_{xx}\right]_f=R''_x$

$$\left[\cancel{\rho_g v(u-u_g)}-\tau_{yx}\right]_f=R''_y$$

$$\left[\cancel{\rho_g w(u-u_g)}-\tau_{zx}\right]_f=R''_z$$

Energy $\left[\rho_g(\cancel{u}h-u_g e)-\cancel{(\tau_{xx}u+\tau_{xy}v+\tau_{xz}w)}+\dot{q}''_x+\sum J_{x,i}h_i\right]_f=\left[-\rho_s u_g e_s+\dot{q}''_x\right]_s$

- Assuming that the velocity of the gas at the wall is negligible

Surface balance equations — Ablating wall

Mass $\left[\rho_{g_i}(u-u_g)+J_{x,i}\right]_f=\left[-\rho_i u_g\right]_s$

Momentum $\left[\rho_g u(u-u_g)+p-\tau_{xx}\right]_f=R_x''$

$\left[\rho_g v(u-u_g)-\tau_{yx}\right]_f=R_y''$

$\left[\rho_g w(u-u_g)-\tau_{zx}\right]_f=R_z''$

Energy $\left[\rho_g(uh-u_g e)-(\tau_{xx}u+\tau_{xy}v+\tau_{xz}w)+\dot{q}_x''+\sum J_{x,i}h_i\right]_f=\left[-\rho_s u_g e_s+\dot{q}_x''\right]_s$

- Assuming that the velocity of the gas at the wall is negligible

Mass $\left[-\rho_{g_i}u_g+J_{x,i}\right]_f=\left[-\rho_i u_g\right]_s$

Momentum $\left[p-\tau_{xx}\right]_f=R_x''$

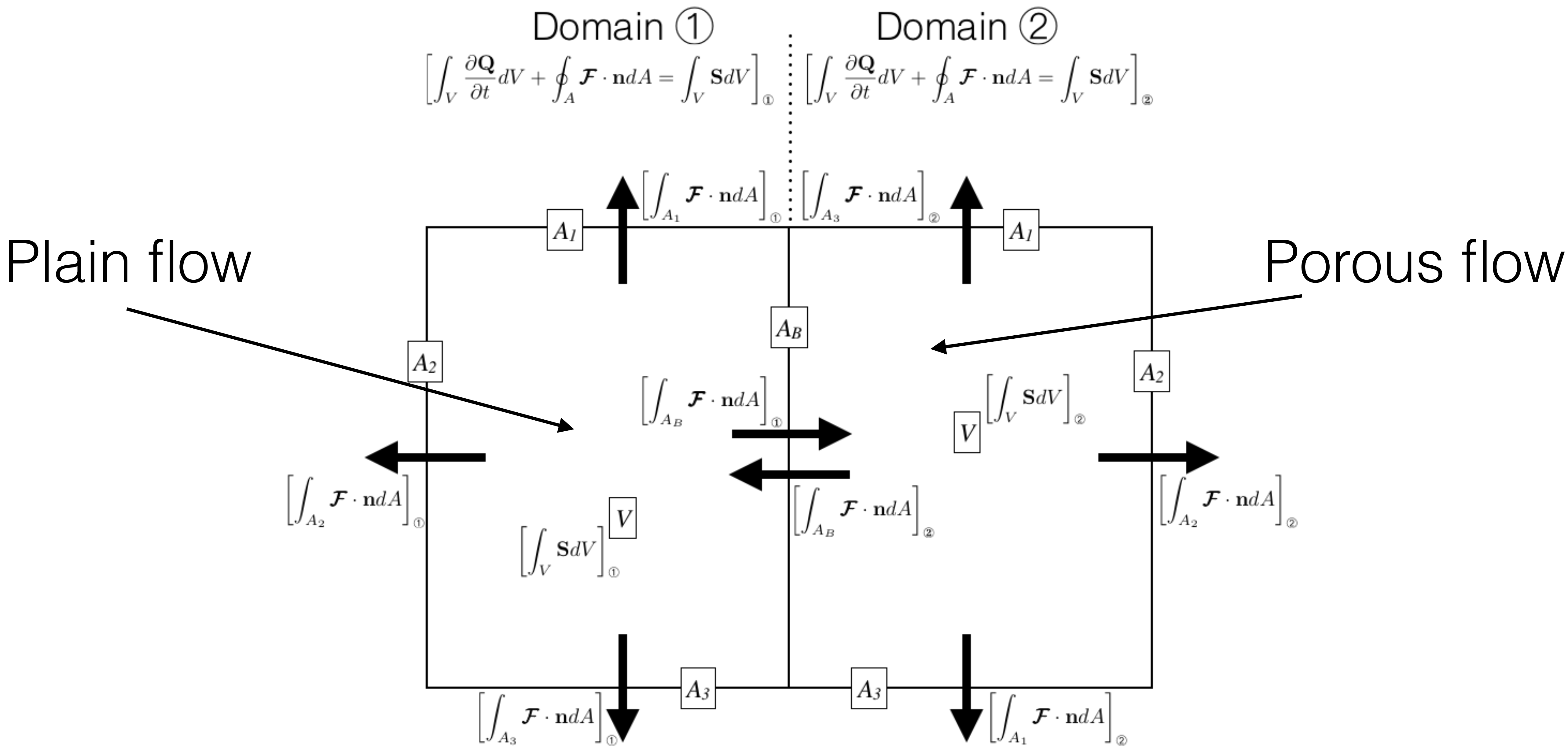
$\left[-\tau_{yx}\right]_f=R_y''$

$\left[-\tau_{zx}\right]_f=R_z''$

Energy $\left[-\rho_g u_g e+\dot{q}_x''+\sum J_{x,i}h_i\right]_f=\left[-\rho_s u_g e_s+\dot{q}_x''\right]_s$

3. Porous interface

- But how to set the condition at the boundary when two different domains are governed by two very different governing equation?
  - For instance, a plain and flow and a porous flow?



[1] Martin, A., Zhang, H., and Tagavi, K. A., "An introduction to a systematic derivation of surface balance equations without the excruciating pain," Int. J. of Heat and Mass Transfer, Vol. 115, Part A, December 2017, pp. 992–999.

Flux matching — Porous interface

	Convective fluxes	Diffusive fluxes
Flow field	$\mathbf{F} = \begin{pmatrix} \rho_1 u & \rho_1 v & \rho_1 w \\ \vdots & \vdots & \vdots \\ \rho_{ngs} u & \rho_{ngs} v & \rho_{ngs} w \\ \rho_g u^2 + p & \rho_g vu & \rho_g wu \\ \rho_g uv & \rho_g v^2 + p & \rho_g wv \\ \rho_g uw & \rho_g vw & \rho_g w^2 + p \\ (E+p)u & (E+p)v & (E+p)w \end{pmatrix},$	$\mathbf{F_d} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{ngs} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \mathbf{q} - \sum_{i=1}^{ngs}(\mathbf{J}_i h_i) & \end{pmatrix}.$
Material	$\mathbf{F} = \begin{pmatrix} \phi\rho_{g_1} u & \phi\rho_{g_1} v & \phi\rho_{g_1} w \\ \vdots & \vdots & \vdots \\ \phi\rho_{g_{ngs}} u & \phi\rho_{g_{ngs}} v & \phi\rho_{g_{ngs}} w \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ \phi\rho_g u^2 + p & \phi\rho_g vu & \phi\rho_g wu \\ \phi\rho_g uv & \phi\rho_g v^2 + p & \phi\rho_g wv \\ \phi\rho_g uw & \phi\rho_g vw & \phi\rho_g w^2 + p \\ \phi\rho_g uH & \phi\rho_g vH & \phi\rho_g wH \end{pmatrix},$	$\mathbf{F_d} = \begin{pmatrix} -\mathbf{J}_1 \\ \vdots \\ -\mathbf{J}_{ngs} \\ \mathbf{0} \\ \\ \mathbf{0} \\ \\ \mathbf{F}_{\text{cond}} \end{pmatrix}.$

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Flux matching — Porous interface

Convective fluxes | Diffusive fluxes

Flow field

$$\mathbf{F} = \begin{pmatrix} \rho_1 u & \rho_1 v & \rho_1 w \\ \vdots & \vdots & \vdots \\ \rho_{ngs} u & \rho_{ngs} v & \rho_{ngs} w \\ \rho_g u^2 + p & \rho_g vu & \rho_g wu \\ \rho_g uv & \rho_g v^2 + p & \rho_g wv \\ \rho_g uw & \rho_g vw & \rho_g w^2 + p \\ (E+p)u & (E+p)v & (E+p)w \end{pmatrix}, \quad \text{Mass} \quad \mathbf{F_d} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{ngs} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \mathbf{q} - \sum_{i=1}^{ngs}(\mathbf{J}_i h_i) & \end{pmatrix}.$$

Material

$$\mathbf{F} = \begin{pmatrix} \phi\rho_{g_1} u & \phi\rho_{g_1} v & \phi\rho_{g_1} w \\ \vdots & \vdots & \vdots \\ \phi\rho_{g_{ngs}} u & \phi\rho_{g_{ngs}} v & \phi\rho_{g_{ngs}} w \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ \phi\rho_g u^2 + p & \phi\rho_g vu & \phi\rho_g wu \\ \phi\rho_g uv & \phi\rho_g v^2 + p & \phi\rho_g wv \\ \phi\rho_g uw & \phi\rho_g vw & \phi\rho_g w^2 + p \\ \phi\rho_g uH & \phi\rho_g vH & \phi\rho_g wH \end{pmatrix}, \quad \text{Mass} \quad \mathbf{F_d} = \begin{pmatrix} -\mathbf{J}_1 \\ \vdots \\ -\mathbf{J}_{ngs} \\ \mathbf{0} \\ \\ \mathbf{0} \\ \\ \mathbf{F}_{\text{cond}} \end{pmatrix}.$$

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Flux matching — Porous interface

Convective fluxes | Diffusive fluxes

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Material

$$\mathbf{F} = \begin{pmatrix} \phi\rho_{g_1} u & \phi\rho_{g_1} v & \phi\rho_{g_1} w \\ \vdots & \vdots & \vdots \\ \phi\rho_{g_{ngs}} u & \phi\rho_{g_{ngs}} v & \phi\rho_{g_{ngs}} w \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ \phi\rho_g u^2 + p & \phi\rho_g vu & \phi\rho_g wu \\ \phi\rho_g uv & \phi\rho_g v^2 + p & \phi\rho_g wv \\ \phi\rho_g uw & \phi\rho_g vw & \phi\rho_g w^2 + p \\ \phi\rho_g uH & \phi\rho_g vH & \phi\rho_g wH \end{pmatrix} \begin{array}{c} \text{Mass} \\ \\ \text{Momentum} \end{array}, \quad \mathbf{F_d} = \begin{pmatrix} -\mathbf{J}_1 \\ \vdots \\ -\mathbf{J}_{ngs} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{F}_{\text{cond}} \end{pmatrix}.$$

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$$\mathbf{F} = \begin{pmatrix} \rho_1 u & \rho_1 v & \rho_1 w \\ \vdots & \vdots & \vdots \\ \rho_{ngs} u & \rho_{ngs} v & \rho_{ngs} w \\ \rho_g u^2 + p & \rho_g vu & \rho_g wu \\ \rho_g uv & \rho_g v^2 + p & \rho_g wv \\ \rho_g uw & \rho_g vw & \rho_g w^2 + p \\ (E+p)u & (E+p)v & (E+p)w \end{pmatrix} \begin{array}{c} \text{Mass} \\ \\ \text{Momentum} \\ \\ \text{Energy} \end{array}, \quad \mathbf{F_d} = \begin{pmatrix} & -\mathbf{J}_1 & \\ & \vdots & \\ & -\mathbf{J}_{ngs} & \\ \tau_{xx} & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \tau_{yy} & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \tau_{zz} \\ & \boldsymbol{\tau}\mathbf{u} - \mathbf{q} - \sum_{i=1}^{ngs} (\mathbf{J}_i h_i) & \end{pmatrix}.$$

Material

$$\mathbf{F} = \begin{pmatrix} \phi\rho_{g_1} u & \phi\rho_{g_1} v & \phi\rho_{g_1} w \\ \vdots & \vdots & \vdots \\ \phi\rho_{g_{ngs}} u & \phi\rho_{g_{ngs}} v & \phi\rho_{g_{ngs}} w \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ \phi\rho_g u^2 + p & \phi\rho_g vu & \phi\rho_g wu \\ \phi\rho_g uv & \phi\rho_g v^2 + p & \phi\rho_g wv \\ \phi\rho_g uw & \phi\rho_g vw & \phi\rho_g w^2 + p \\ \phi\rho_g uH & \phi\rho_g vH & \phi\rho_g wH \end{pmatrix} \begin{array}{c} \text{Mass} \\ \\ \\ \text{Momentum} \\ \text{Energy} \end{array}, \quad \mathbf{F_d} = \begin{pmatrix} -\mathbf{J}_1 \\ \vdots \\ -\mathbf{J}_{ngs} \\ \mathbf{0} \\ \mathbf{0} \\ \mathbf{F}_{\text{cond}} \end{pmatrix}.$$

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Surface energy balance — Porous interface

- Therefore, the fluxes simply need to be evaluated at the same surface, using the contribution from both sides, and solved for the primitive variable (y_i, u, v, w, T)

$$[\mathbf{F} + \mathbf{F_d}]_{\text{flow}} \cdot \hat{\mathbf{n}} = [\mathbf{F} + \mathbf{F_d}]_{\text{material}} \cdot \hat{\mathbf{n}}$$

- For instance, using the energy fluxes, and assuming that the surface is perpendicular to *x-dir*

$$(E + P)u + \boldsymbol{\tau}_{xi} \cdot \mathbf{u} - q_x + \sum_{i=1}^{ngs} (J_{xi} h_i) = \phi \rho u H + q_{\text{cond}}$$

$$k_T \frac{\partial T}{\partial \eta} + k_V \frac{\partial T_V}{\partial \eta} + \sum_{i=1}^{N_c} \rho h_i D \frac{\partial y_i}{\partial \eta} = q_{\text{cond}} + \dot{m}_{sw}(h_w - h_{sw})$$

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Surface mass balance — Porous interface

- And using the mass fluxes

$$\left[\dot{m}''Y_i - \rho_g D \frac{\partial Y_i}{\partial x}\right]_f = \left[\dot{m}''Y_i - \rho_g D \frac{\partial Y_i}{\partial x}\right]_p$$

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Surface momentum balance — Porous interface

- And using the momentum fluxes

$$\left[\rho_g u^2 + p - \tau_{xx}\right]_f = \left[\phi \rho_g u^2 + p - \alpha_s \phi \mu \frac{2u}{\sqrt{K_{xx}}}\right]_p$$

$$\left[\rho_g u v - \tau_{yx}\right]_f = \left[\phi \rho_g v u - \alpha_s \phi \mu \left(\frac{v}{\sqrt{K_{xx}}} + \frac{u}{\sqrt{K_{yy}}}\right)\right]_p$$

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- Very far from $p_f = p_p$

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Surface balance equations — Porous interface

- We can clearly see that some terms have been omitted
  - shear friction in the energy
  - species diffusion in the material side
  - the whole momentum balance equation, is simplified to equal pressure
- The flux matching method, on the other hand, is rigorous, and consistent with the equation solved in the code: if a term is omitted in governing equations, it will automatically be omitted in the surface balance equations

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4. Flow over a porous medium

- For a flow over a surface, the momentum surface balance equations can be reduced to

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- For a flow over a surface, the momentum surface balance equations can be reduced to
  - Assuming a two-dimensional flow
  - Assuming a Stokes flow on one side, and Darcy's Law for on the other
  - Assuming that the fluid flows parallel to the wall, then $u=0$

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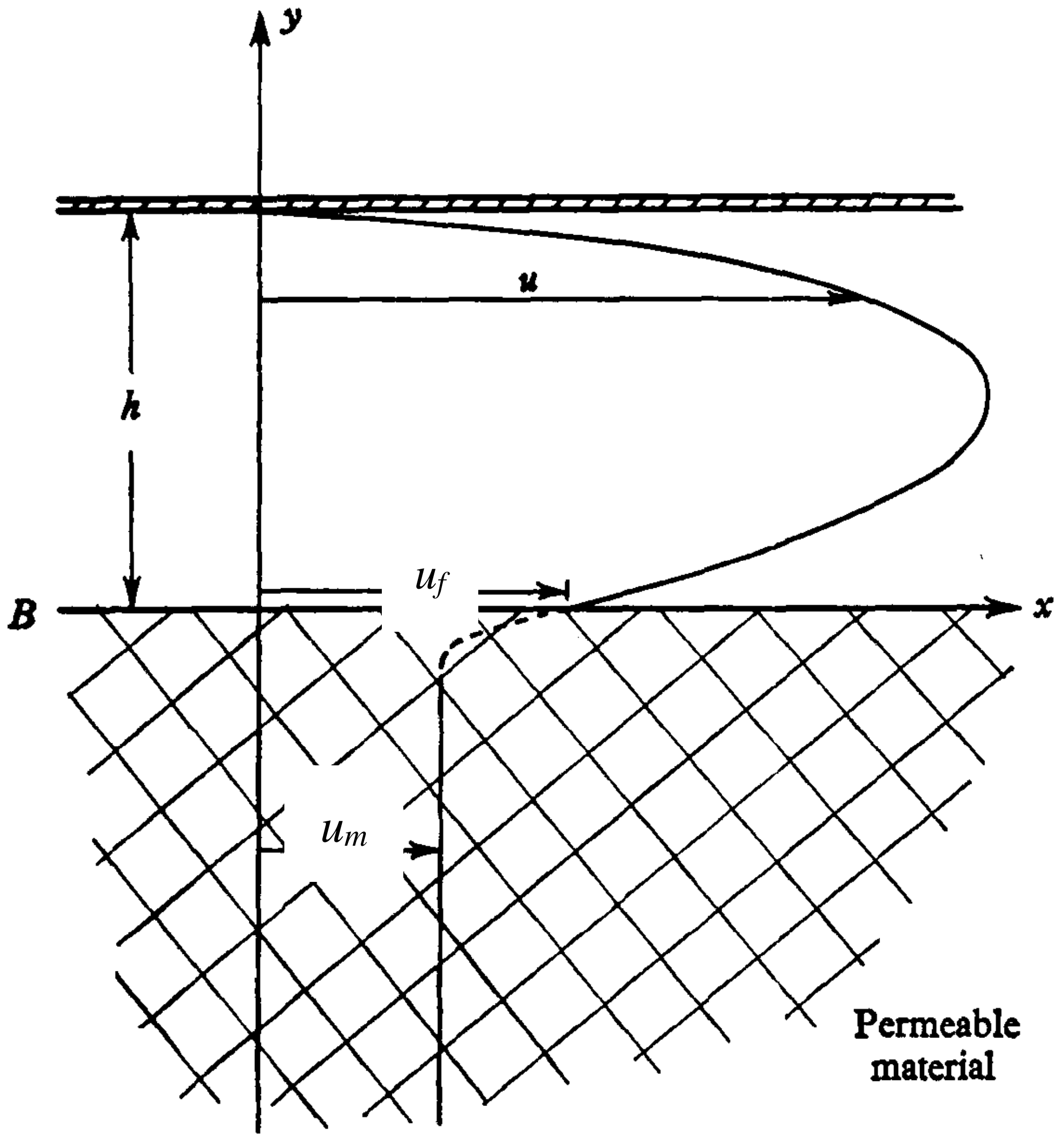

$$\frac{\partial u_f}{\partial y} = -\frac{\alpha_s}{\sqrt{K}} u_p$$

$$p_f = p_p$$

Beaver-Joseph condition

[1] Beavers, G. S. and Joseph, D. D., "Boundary conditions at a naturally permeable wall," Journal of Fluid Mechanics, Vol. 30, No. 01, October 1967, pp. 197–207.

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Remarks

- Complex boundary conditions need not be derived one at a time, a process that is time consuming and ''painful''*
- A systematic and universal method of matching governing equations at the boundaries and interfaces can provide a rigorous approach that can consistently result in the correct set of boundary and interface conditions
- The method presented here results in an accurate and useful set of boundary and interface conditions

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- However, implementing these BC in a code still requires a lot of work….

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